ICSET 2026

2nd International Congress on Sustainable Energy and related Technologies

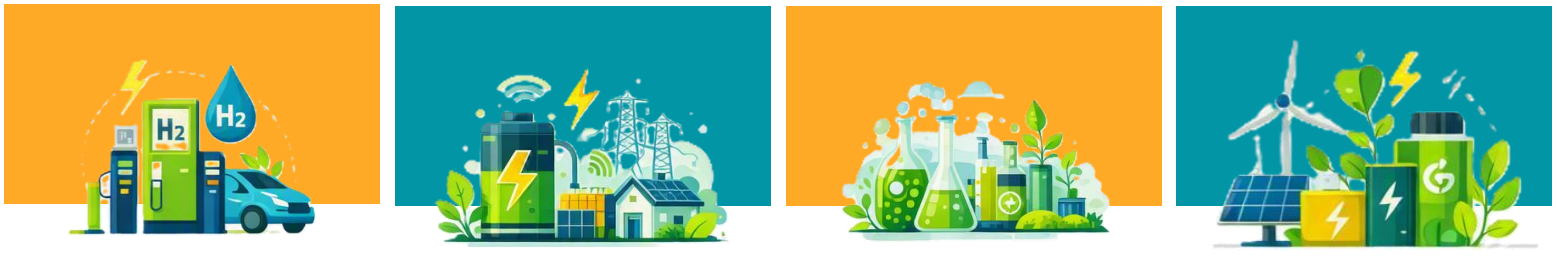
Palermo (Italy), August 31 - September 4, 2026

BOOK OF ABSTRACTS



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Hyland Enterprise



Save the Planet, Enjoy your Life!



MESSAGE FROM THE ORGANISERS

Dear Participants,

It is with great pleasure that we welcome you to the 2nd International Congress on Sustainable Energy and Related Technologies (ICSET 2026), hosted in the extraordinary city of Palermo, a crossroads of cultures and history that offers an inspiring backdrop for a congress devoted to building a sustainable energy future.

The transition toward a clean and secure energy system is among the defining challenges of our time, calling for solutions that are technically sound, economically viable, and socially fair. Meeting it requires the exchange of ideas across disciplines and borders, and ICSET 2026 was conceived as precisely such a space a forum spanning hydrogen and energy conversion, chemical and thermal storage, green chemistry, and emerging technologies.

This Book of Abstracts gathers the knowledge, creativity, and commitment of researchers and innovators from around the globe. Each contribution represents not merely a scientific result but a concrete step toward a cleaner and more resilient world.

Our motto, "Save the planet, enjoy your life", captures the essence of this vision. Sustainability is too often framed as sacrifice; we believe the opposite is true. The responsible use of energy and resources is an opportunity to enhance our quality of life while safeguarding the wellbeing of future generations. Protecting the planet and enjoying life are not competing goals, but two sides of the same commitment.

We sincerely thank you for your contributions and participation. May our time in Palermo be a source of inspiration, meaningful dialogue, and lasting impact.

Sincerely,

The Organising Committee ICSET 2026,

Claudia D'Urso, Cristina Italiano, Stefano Trocino, Antonio Vita



Contents

Organising Committee 16
International Advisory Board 17
Scientific Committee 18
Technical Committee 18
Local Committee 19
Plenary 20
Sponsorship 24
Supporting Companies 24
Supporting Projects & Association 25
Endorsers 25
Satellite Events 26
RISEnergy – Project 27
IAGE- Italy - Round Table 30
RdS 25-27- Special Sessions 32
Abstracts 34
Plenary 34
HIGH SUSTAINABILITY AND ENVIRONMENTAL REQUIREMENTS FOR BATTERIES AND BATTERY SAFETY - (P001) 35
TANDEM CATALYSIS: ONE-POT SAF SYNTHESIS FROM CO_2 – (P002) 37
REDOX-MEDIATED ELECTROSYNTHESIS OF AMMONIA FROM RENEWABLES - (P003) 39
Oral 40
SHUNT, PARASITIC AND REVERSE CURRENTS IN BIPOLAR ELECTRODE STACKS – (C001) 41
SYNTHESIS AND CHARACTERIZATION OF PELLETIZED PEROVSKITES FOR GREEN HYDROGEN PRODUCTION BY TWO-STEP THERMOCHEMICAL WATER SPLITTING CYCLE – (C006) 42



ACTIVITY-STRUCTURE DEPENDANCE ON SURFACE CRYSTAL PHASE OF ALLOY Pd-Cu NANOPARTICLES FOR THE HYDROGEN OXIDATION REACTION – (C008) 44

OPERANDO DRIFT INVESTIGATION OF CU-BASED CATALYSTS DURING CO_2 CONVERSION TO METHANOL IN PRESENCE OF GREEN HYDROGEN – (C009) 46

EFFECT OF CONVENIENTLY FUNCTIONALIZED NANOMATERIALS ON ANION EXCHANGE MEMBRANES FOR WATER ELECTROLYSIS – (C010) 48

SUSTAINABLE HYDROGEN UPGRADING FROM SYNGAS THROUGH ULTRA-MICROPOROUS CARBON HOLLOW FIBER MEMBRANES – (C011) 50

ELECTRIFIED SORPTION-ENHANCED CATALYTIC DRY REFORMING OF METHANE FOR CLEAN HYDROGEN PRODUCTION – (C012) 52

FROM CO_2 TO POWER: ASSESSING THE ENVIRONMENTAL IMPACTS OF POTASSIUM FORMATE AS CHEMICAL ENERGY CARRIER – (C014) 54

SO-FREE: FROM SYSTEM ARCHITECTURE TO COMMISSIONING OF A MULTI-FUEL SOFC PLATFORM – (C015) 56

Ni EXSOLUTION AND DEFECT CHEMISTRY OF La(Sr)Mn(Ni,Cr)O_3 FOR SOFC AND SOEC ELECTRODES – (C016) 58

HIGH-ENTROPY OXIDES WITH SACRIFICIAL HIGH-VALENCE METALS TO OBTAIN EFFICIENT AND STABLE ELECTROCATALYSTS FOR WATER OXIDATION IN AEM ELECTROLYZERS – (C018) 60

TAILORING ANODIZED WO_3 NANOSTRUCTURES FOR PHOTOELECTROLYSIS OF BIOMASS CONTAINING SOLUTIONS AND PHOTOCATALYTIC AIR PURIFICATION – (C019) 62

STABILITY ENHANCEMENT IN METHANOL-TO-DME CATALYTIC MEMBRANE CONTACTORS ENABLED BY BILAYER ZSM-5 MEMBRANES - (C020) 64

THROUGH-FLOW CATALYTIC MEMBRANE CONTACTORS FOR INTENSIFIED DIMETHYL ETHER SYNTHESIS: COMPARISON BETWEEN BEA ZEOLITE AND γ-Al_2O_3 MEMBRANES – (C021) 66

ADVANCING THERMAL ENERGY STORAGE SYSTEMS: PROGRESS OF THE ECHO PROJECT – (C022) 68

DEVELOPMENT OF HIGHLY SELECTIVE MULTICHANNEL CARBON MOLECULAR SIEVE MEMBRANES FOR HYDROGEN PURIFICATION – (C024) 70



CO_2 VALORIZATION INTO SYNTHETIC METHANE BY AN INTEGRATED CO_2-METHANATION REACTOR COMBINED WITH A BIO-POLYMERIC MEMBRANE SEPARATION SYSTEM: AN EXPERIMENTAL STUDY COMBINED TO EXERGY AND COST ANALYSES – (C025) 72

IN OPERANDO HIGH-RESOLUTION LI DEPTH PROFILING IN A THIN-FILM ALL-SOLID-STATE BATTERY USING TOF-ERDA AND NEUTRON DEPTH PROFILING – (C027) 74

ENHANCING EFFICIENCY AND PROCESS OPTIMIZATION USING OPENFOAM THREE-DIMENSIONAL SIMULATION FOR INDUCTION HEATING – (C031) 75

IMPROVED ELECTROLYTIC CELL PERFORMANCE USING LASER-TEXTURED Ni-FELT – (C032) 77

3D MULTIPHYSICS MODELING OF REVERSIBLE SOLID OXIDE BOTTOM CELL – (C036) 79

EXPERIMENTAL ASSESSMENT AND SYSTEM-LEVEL ANALYSIS OF ALUMINUM-BASED HYDROGEN STORAGE – (C037) 81

ZEOLITE-TEMPLATED CARBONS AS EFFECTIVE SUPPORTS FOR BOOSTING COPPER CATALYST FUNCTIONALITY IN CO_2-TO-METHANOL PRODUCTION – (C038) 83

A DUAL SUSTAINABILITY PERSPECTIVE ON PHOTOELECTROLYSIS: INTEGRATED ENVIRONMENTAL AND ECONOMIC LIFE CYCLE ASSESSMENT OF GREEN HYDROGEN PRODUCTION – (C044) 85

CATALYTIC DEHYDROGENATION-HYDROGENATION OF ORGANIC CARRIERS FOR CLEAN HYDROGEN GENERATION AND STORAGE: EXPLOITATION OF DIFFERENT BIO-MOLECULES AND CATALYST OPTIMIZATION – (C047) 87

SCALABLE PRODUCTION OF Pt CATALYST EMBEDDED IN NANOSCALE CARBON NETWORK FOR DURABLE FUEL CELLS – (C048) 89

SUSTAINABLE AQUEOUS SYNTHESIS OF MIL-100(Fe): A PROMISING MOF FOR WATER SORPTION APPLICATIONS – (C049) 91

PGM-FREE METAL-FUNCTIONALIZED TIO_2 NANOTUBES ELECTRODES FOR ALCOHOL OXIDATION TOWARD COUPLED GREEN HYDROGEN AND VALUE-ADDED CHEMICALS PRODUCTION – (C052) 93

LANAR CELL DESIGN FOR IMPROVED PERFORMANCE OF $NaI–AlCl_3$ EUTECTIC-BASED MOLTEN SODIUM BATTERIES – (C053) 95



ADVANCING PLANAR NASICON BATTERIES THROUGH NI–FE COMPOSITES FOR IMPROVED PERFORMANCE UNDER MILD THERMAL CONDITIONS - (C054) 97

FIRST PRINCIPLES CALCULATIONS OF $SrTiO_3$ ENGINEERING WITH Bi BASED HETEROSTRUCTURES FOR EFFICIENT PHOTOSTIMULATED HYDROGEN PRODUCTION - (C056) 99

HIGH ACTIVE-MASS FREE-STANDING $Na_4MnCr(PO_4)_3$/CNF CATHODES FOR SODIUM-ION BATTERIES - (C057) 101

DOUBLE SUBSTITUED Co-FREE PEROVSKITE OXIDES FOR REVERSIBLE SOLID OXIDE CELLS ($RSOC_S$) - (C058) 103

INTEGRATED SYSTEM ANALYSIS OF BIOGAS-TO-METHANOL PRODUCTION WITH UPSTREAM CO_2 CAPTURE BY CALCIUM LOOPING AND CERIA-BASED CHEMICAL LOOPING SYNGAS GENERATION - (C060) 105

DENSITY FUNCTIONAL THEORY CALCULATIONS ON G-C3N4/SRTIO3 HETEROSTRUCTURE - (C061) 107

PERFORMANCE AND DURABILITY IMPROVEMENT OF LSCF ELECTRODE FOR SOLID OXIDE ELECTROLYSIS - (C063) 109

NEW ENVIRONMENTALLY FRIENDLY MECHANOCHEMICAL SYNTHESIS OF Cu-BASED CATALYSTS FOR E-METHANOL PRODUCTION - (C064) 111

ENGINEERING 2D $SRTIO_3$ NANOSTRUCTURES FOR ENHANCED PHOTOCATALYTIC H_2 EVOLUTION THROUGH AURIVILLIUS-PHASE $Bi_4Ti_3O_{12}$ TRANSFORMATION - (C071) 113

ELECTRIFIED MEMBRANE REACTOR FOR NH_3 DECOMPOSITION: COMBINING H_2 SCAVENGING AND EFFECTIVE HEAT SUPPLY - (C072) 115

CFD STUDY OF AMMONIA SYNTHESIS AND CRACKING IN MEMBRANE REACTOR WITH PERIODIC OPEN CELLULAR STRUCTURE, FOR LONG-TERM HYDROGEN STORAGE - (C073) 117

PLATINUM BASED CATHODE FOR HYDROGEN PRODUCTION THROUGH PLASMA-BASED SYNTHESIS - (C074) 119

$NiFe_2O_4$ AS AN EFFICIENT AND STABLE ANODE FOR AEM WATER ELECTROLYSERS - (C075) 122

ENVIRONMENTAL ANALYSIS OF A NANOWIRE LEAD-ACID BATTERY CELL - (C076) 124



ROBUST Fe/C CATALYSTS FROM SIMPLE PREPARATION FOR STABLE AMMONIA DECOMPOSITION - (C078) 126

KINETIC AND MECHANISTIC STUDY OF NH_3 DECOMPOSITION OVER HIGHLY ACTIVE Ru/CeO_2 CATALYSTS - (C079) 128

INVESTIGATION OF STEAM-IRON PROCESS FOR HYDROGEN STORAGE OVER FUSED Fe-BASED MATERIALS - (C080) 130

ELECTRIFIED REVERSE WATER GAS SHIFT: AN EXPERIMENTAL AND MODELLING STUDY ON A JOULE-HEATED PACKED FOAM REACTOR. - (C082) 132

ENERGY AND ENVIRONMENTAL PERFORMANCE ASSESSMENT OF A BIO-BASED ELECTRODE MANUFACTURING FOR VANADIUM REDOX FLOW BATTERY - (C083) 134

SCALABLE ELECTROSPINNING SYNTHESIS OF CUO AND Fe_2O_3 ELECTRODES FOR PHOTOELECTROLYSIS - (C084) 136

EMERALD: MODELING AND EXPERIMENTAL VALIDATION OF A NOVEL RADIAL-CURRENT EREACTOR FOR INTENSIFIED ENDOTHERMIC CATALYTIC PROCESSES - (C086) 138

FLUORINE-FREE POLYMER ELECTROLYTE MEMBRANE FOR ADVANCED HIGH-ELECTROCHEMICAL PERFORMANCES 2 V SOLID-STATE ASYMMETRIC SUPERCAPACITOR - (C087) 140

VALORIZATION OF SALTWORKS BITTERN FOR $Mg(OH)_2$ PRODUCTION: A LIFE CYCLE ASSESSMENT - (C091) 143

$La(OH)_3$-IROX CATALYSTS FOR EFFICIENT OXYGEN EVOLUTION REACTION IN ACIDIC ENVIRONMENT - (C092) 145

CO_2-TO-METHANOL SYNTHESIS: EXPERIMENTAL, MODELING, AND PROCESS ASSESSMENT OF Cu-, In-, AND ZnZr-BASED CATALYSTS - (C093) 147

GASIFICATION OF PLASTIC WASTE WITH OXYGEN AND STEAM IN A LARGE PILOT SCALE GASIFIER - (C094) 149

VOLCANIC ASH AS SUSTAINABLE INORGANIC SUPPORT FOR SUPERCAPACITORS ELECTRODES - (C095) 151

BIO-FUNCTIONALIZED ELECTROSPUN MULTILAYER MEMBRANES AND SUSTAINABLE AQUEOUS ELECTRODES FOR LITHIUM-ION BATTERIES - (C096) 153



EFFECT OF PHOSPHORUS CONTENT IN Ni CATALYSTS SUPPORTED ON ACTIVATED CARBONS DERIVED FROM RESIDUAL BIOMASS IN CO_2 HYDROGENATION - (C097) 155

SOLAR HYDROGEN PRODUCTION VIA METHANE CHEMICAL LOOPING CYCLES USING A γ-Al_2O_3 SUPPORTED PEROVSKITE CATALYST - (C098) 157

SERP METHANOL SYNTHESIS FROM CO_2/H_2: FROM EXPERIMENT TO SIMULATION TO OPTIMIZE AN INTENSIFIED PROCESS - (C099) 160

QUANTIFYING THE IMPACT OF WASTE HETEROGENEITY ON GASIFICATION PERFORMANCE: A DEEP LEARNING-BASED SURROGATE MODELING APPROACH FOR SYNGAS AND TAR PREDICTION - (C100) 162

A REDUCED-PHYSICS 3D CFD MODEL FOR FIELD-DRIVEN DESIGN OF TPMS FLOW FIELDS IN PEMFC BIPOLAR PLATES - (C103) 163

TRUE OR FALSE? THE THREAT OF FAKE SCIENTIFIC INFORMATION - (C104) 166

EXPLORING THE EFFECT OF CE AND CU DOPING ON Ni/MgO CATALYSTS FOR CH_4 DRY REFORMING AND CH4 ACTIVATION - (C105) 168

FABRICATION OF STRUCTURED COMPOSITE PHOTOCATALYTIC MEMBRANES: FROM HOLLOW FIBER ENGINEERING TO REACTOR IMPLEMENTATION IN WATER TREATMENT - (C107) 170

KAPMEMLYSE:INTEGRATING CAPILLARY FEEDING AND AEM TECHNOLOGY FOR EFFICIENT, NOBLE METAL FREE HIGH PRESSURE WATER ELECTROLYSIS - (C114) 172

WATER-BASED EXTRUDED LFP AND NMO ELECTRODES FOR SUSTAINABLE SIB AND NIB - (C115) 174

PERFORMANCE EVALUATION OF STRUCTURED POCS CATALYSTS FOR HYDROGEN PRODUCTION VIA AMMONIA DECOMPOSITION - (C116) 176

HUMAN-ROBOT COLLABORATIVE ASSEMBLY AND QUALITY ASSURANCE IN PROTON EXCHANGE MEMBRANE FUEL CELLS - (C120) 178

SUSTAINABLE SYSTEMS: AN ADAPTIVE MANAGEMENT FRAMEWORK FOR PLANNING, PERFORMANCE, REPORTING AND STRATEGIC ORIENTATION - (C121) 180

BIO-INSPIRED ELECTROCHEMICAL SYSTEMS FOR SUSTAINABLE HYDROGEN ACROSS THE VALUE CHAIN - (C122) 182



INNOVATIVE FUNCTIONAL GROUPS TO IMPROVE THERMAL DURABILITY AND PERFORMANCE OF ANION EXCHANGE MEMBRANES FOR GREEN HYDROGEN PRODUCTION - (C124) 184

WASTE DERIVED MOS_2 NANOSTRUCTURES FOR HIGH-PERFORMANCE SUPERCAPACITORS - (C125) 186

DUAL-FUNCTION MATERIALS FOR LOW-TEMPERATURE INTEGRATED CO_2 CAPTURE/METHANATION - (C126) 188

POLYBENZIMIDAZOLES ARCHITECTURES FOR HIGH-TEMPERATURE PROTON-EXCHANGE MEMBRANES - (C127) 190

INSIGHTS INTO THE RECONSTRUCTION OF MIXED OXIDES DURING ACIDIC OER - (C129) 192

MODELLING OF A GAS TRANSMISSION NETWORK FOR HYDROGEN INJECTION: - (C130) 194

WHITE HYDROGEN IN THE ENERGY TRANSITION: TECHNICAL CHALLENGES AND RESEARCH FRONTIERS - (C131) 196

RECYCLING PROCESSES FOR SOLID OXIDE ELECTROLYSIS CELLS - (C132) 198

ARCHITECTED 3D-PRINTED FUEL CELLS AND NEXT-GENERATION CERAMIC ENERGY PLATFORMS - (C133) 200

AMMONIA AS A H_2 CARRIER: ADVANCES IN NH_3 DECOMPOSITION TECHNOLOGIES AND INTEGRATION IN THE GREEN VALUE CHAIN - (C134) 202

HIGH-TEMPERATURE ENERGY STORAGE VIA REACTION CYCLES INVOLVING THE USE OF THERMO-CHEMICAL MATERIALS IN FLUIDIZED BEDS. - (C135) 204

HYDROGEN AND HIGH-ADDED VALUE PRODUCTION THROUGH AN INNOVATIVE BORATE-BOOSTED BIO-ALCOHOL UPGRADING - (C136) 206

MEDIUM-TEMPERATURE ENERGY STORAGE SYSTEMS USING CONCRETE AND PHASE CHANGE MATERIALS. - (C137) 208

THE ROLE OF ELECTRICITY STORAGE IN THE FUTURE ITALIAN ENERGY SCENARIOS - (C138) 210



CONTROLLED THERMAL OXIDATION OF $Ti_3Al(1-X)TmxC_2$ (TM = Sn, Si) MAX PHASES FOR THE DEVELOPMENT OF NANOSTRUCTURED LI/NA-ION BATTERY ANODES - (C140) 213

COUPLED ATES–DHN SIMULATIONS: ASSESSING THE IMPACT OF HYDROGEOLOGICAL, THERMAL AND ENERGY PARAMETERS ON INTEGRATED SYSTEM PERFORMANCE - (C143) 215

CLOSED-VESSEL EXPLOSION OF AMMONIA–HYDROGEN MIXTURES IN AIR - (C145) 217

ACTIVE MATERIALS FOR BIOFUEL CONVERSION IN HIGH TEMPERATURE ELECTROCHEMICAL CELLS - (C149) 219

ELECTROCHEMICAL WATER OXIDATION FOR IN-ORBIT HYDROGEN PEROXIDE PRODUCTION - (C150) 221

ENERGY CONSUMPTION ANALYSIS AND LIFE CYCLE ASSESSMENT OF A LI-ION BATTERY PACK FOR A LOWER-LIMB ASSISTIVE EXOSKELETON - (C151) 223

STOICHIOMETRIC CONTROL OF CO-SPUTTERED $BiVO_4$ THIN FILMS FOR ENHANCED PHOTOELECTROCHEMICAL WATER OXIDATION - (C154) 225

FUNCTIONALIZED MEMBRANES BASED ON POLY(2,6-DIMETHYL-1,4-PHENYLENE)OXIDE (PPO) - (C155) 227

EUROPEAN PROJECT FUNDED C3POE : SUSTAINABLE PLUG & PLAY WATER ELECTRICITY COUPLING FOR ISLANDS AND ISOLATED COASTAL SITES OPTIMAL DESIGN OF AN OFF-GRID HYBRID RENEWABLE ENERGY SYSTEM INVOLVING BATTERIES, HYDROGEN AND PRODUCING WATER AND ELECTRICITY - (C161) 232

WASTE-TO-FUEL: EFFICIENT CONVERSION OF PLASTIC WASTE TO METHANE VIA CATALYTIC HYDROGASIFICATION IN AN OPTIMIZED REACTOR CONFIGURATION - (C163) 234

NEAR-AMBIENT CO_2 ACTIVATION WITH ULTRA-HIGH METHANE SELECTIVITY - (C164) 236

DIMENSIONLESS FRAMEWORK FOR CO_2 SPLITTING IN DBD PLASMA REACTORS - (C165) 238

METHANOL PRODUCTION FROM CO_2 HYDROGENATION OVER Cu SUPPORTED ON BLACK-TiO_2 - (C166) 240

AMMONIA CRACKING ELECTRIFIED STRUCTURED REACTOR COUPLED WITH PEM FUEL CELL FOR POWER GENERATION - (C167) 242



HYDROGEN PRODUCTION VIA AMMONIA CRACKING REACTION: IMPACT OF SUPPORT MATERIAL ON CATALYTIC PERFORMANCE - (C168) 244

ENHANCING SELECTIVITY TO PROPYLENE IN THE PROPANE DEHYDROGENATION PROCESS BY JOULE-HEATED PT-SN BASED CATALYTIC FOAMS - (C169) 246

LOW TEMPERATURE H_2 PRODUCTION BY HLC CRACKING IN ELECTRIFIED STRUCTURED REACTORS INTEGRATED WITH SUPPORTED Pd MEMBRANE - (C171) 248

COST AND ROBUSTNESS OF OPTIMIZED CROSS-MEDITERRANEAN GREEN–BLUE HYDROGEN SUPPLY CHAINS UNDER 2050 POLICY SCENARIOS - (C174) 250

Ni ALLOY NANOWIRE ELECTRODES INTEGRATED IN A ZERO-GAP ALKALINE WATER ELECTROLYZER - (C175) 254

METHANE CHEMICAL LOOPING OVER NI-BASED OXYGEN CARRIERS FOR SUSTAINABLE HYDROGEN PRODUCTION - (C176) 256

EFFECT OF BALANCE-OF-PLANT DESIGN PARAMETERS ON THE LOAD-DEPENDENT SPECIFIC ENERGY CONSUMPTION OF PEM WATER ELECTROLYZER - (C178) 258

ERA JOINT PROGRAMME ON ENERGY STORAGE (C182) 260

BALTICSEAH_2: DEMONSTRATING HYDROGEN ECONOMY WITH THE LARGEST CROSS-BORDER HYDROGEN VALLEY IN EUROPE, BUILDING UP THE VISION - (C185) 261

BEST PRACTICES FOR SCIENTIFIC MANUSCRIPT PREPARATION AND ETHICAL USE OF AI TOOLS - (C179) 263

PILOT-SCALE SYNGAS UPGRADING BY TWO-STAGE CATALYTIC TAR CRACKING BASED ON DOLOMITE AND NI/ALUMINA - (C186) 264

NEW COMPOSITE ADSORBENTS FOR THERMOCHEMICAL HEAT STORAGE - (C193) 266

ENERGY STORAGE INNOVATION IN ITALY: BATTERY TECHNOLOGY EVOLUTION AND THE "RICERCA DI SISTEMA" PROGRAMME – (C194) 267

POLISHING METHANE-CONTAINING GAS STREAMS TO NATURAL GAS GRID SPECIFICATIONS USING ALUMINA-CARBON MOLECULAR SIEVE MEMBRANES - (C196) 269



EUROPEAN VISION AND STRATEGIC RESEARCH AND INNOVATION AGENDA FOR THE BATTERY SECTOR: STATE OF PLAY AND FUTURE ACTIONS OF THE SET PLAN IMPLEMENTATION WORKING GROUP - (C197) 271

LOW-TRANSITION-TEMPERATURE ELECTROLYTES FOR RECHARGEABLE ZINC BATTERIES - (C199) 272

SUSTAINABLE ENERGY STORAGE: ASSESSING INNOVATIVE MATERIALS THROUGH LIFE CYCLE ASSESSMENT – (C200) 274

CEETe H_2: AN INTEGRATED PLATFORM FOR HYDROGEN TECHNOLOGIES – (C204) 276

Poster 278

HARNESSING LOW-VELOCITY TIDAL CURRENTS: DUCT-OPTIMIZED TURBINES AND DIVER-LESS MAINTENANCE FOR BRIDGE-INTEGRATED POWER – (C002) 279

CATHODE MATERIALS AND ELECTROLYTE FORMULATIONS FOR EMERGING POTASSIUM-SULFUR BATTERIES – (C003) 281

EFFICIENT MOF-BASED CATALYSTS FOR THE DIRECT SYNTHESIS OF DIMETHYL CARBONATE (DMC) FROM CO_2 AND METHANOL – (C013) 283

POSSIBILITY OF STEAM ELECTROLYSIS IN DOUBLE SIDED SOLID OXIDE CELLS – (C033) 286

FROM PHOTOVOLTAICS TO HYDROGEN TECHNOLOGIES: A UNIVERSAL LSTM-BASED MODEL FOR MARKET DEVELOPMENT FORECASTING – (C034) 288

HIGH-PURITY HYDROGEN PRODUCTION FROM AMMONIA USING 290

INTEGRATED PD–AG MEMBRANE REACTORS WITH STRUCTURED CATALYSTS – (C039) 290

MULTICRITERIA DECISION ANALYSIS METHODOLOGIES: A REVIEW APPLIED TO THE ENERGY SECTOR – (C043) 292

A DUAL SUSTAINABILITY PERSPECTIVE ON PHOTOELECTROLYSIS: INTEGRATED ENVIRONMENTAL AND ECONOMIC LIFE CYCLE ASSESSMENT OF GREEN HYDROGEN PRODUCTION – (C044) 295

MACHINE LEARNING-BASED CONTROL OF A SOFC SYSTEM UNDER VARIABLE LOAD CONDITIONS – (C045) 297



DESIGN AND VALIDATION OF A 10 CM² TANDEM PHOTOELECTROCHEMICAL PROTOTYPE FOR WATER SPLITTING USING NON-CRITICAL RAW MATERIALS – (C046) 299

REALIZATION AND EXPERIMENTAL VALIDATION OF A PEM FUEL CELL STACK OPERATING WITH OXYGEN-ENRICHED FOR NAVAL APPLICATIONS - (C050) 301

VIRTUAL ASSEMBLY OF A PEMFC STACK FOR MARINE APPLICATIONS WITH OXYGEN-ENRICHED SIMULATED AIR – (C051) 303

ENVIRONMENTAL ASSESSMENT OF THE MANUFACTURING PHASE OF AN INNOVATIVE SOFC SYSTEM FED WITH AMMONIA - (C055) 305

UNDERGROUND HYDROGEN STORAGE IN DEEP SALINE AQUIFERS: A GEOLOGICAL FEASIBILITY STUDY FOR THE ITALIAN CONTEXT - (C059) 307

SEA PLANT DERIVED BIOCARBON AS ELECTROCATALYSTS SUPPORT FOR DMFC - (C065) 309

SUSTAINABLE MATERIALS FOR HYDROGEN PRODUCTION VIA TANDEM PHOTOELECTROLYSIS AND ALKALINE ELECTROLYSIS - (C067) 311

ASSESSING ENERGY RESILIENCE OF BUILDINGS AND DISTRICTS UNDER HEATWAVE SCENARIOS: THE CASE OF MONREALE – (C068) 313

INTEGRATED VOC OXIDATION AND THERMO/PHOTOTHERMO METHANE REFORMING OVER NI/GD-ZR-MODIFIED CERIA - (C070) 315

PYRAZOLE- AND TETRAZOLE-BASED CONDUCTING SALTS FOR SIB ELECTROLYTES - (C077) 317

CRYSTAL PHASE EVOLUTION OF THIN FILMS OF Fe_2O_3 - (C085) 319

ENGINEERING BIOCHAR AS A DUAL-FUNCTION CARBON PLATFORM FOR SODIUM/LITHIUM STORAGE AND ELECTROCHEMICAL SENSING - (C101) 321

LOW-COST TI-DOPED HEMATITE AND $CU_2CR_2O_5$ PHOTOELECTRODES FOR TANDEM PHOTOELECTROCHEMICAL HYDROGEN PRODUCTION - (C106) 323

DIGITAL TWIN FRAMEWORK FOR PRE-DEPLOYMENT PLANNING OF THE H2TALENT GREEN HYDROGEN VALLEY IN ALENTEJO - (C108) 325

STRUCTURE-ACTIVITY RELATIONSHIPS IN Mg-DOPED $LaNiO_3$-DERIVED CATALYSTS FOR LOW-TEMPERATURE AMMONIA DECOMPOSITION - (C109) 327



SYNTHESIS AND CHARACTERIZATION OF NASICON-BASED ELECTROLYTES DOPED WITH TRANSITION METALS - (C110) 329

MARKET-DRIVEN ROLLING DAY-AHEAD OPTIMIZATION OF HYDROPOWER REVENUES THROUGH FLEXIBLE ELECTRICITY AND HYDROGEN PRODUCTION – (C111) 331

EFFECT OF REACTION PARAMETERS ON CRACKING AND SELECTIVE CATALYTIC DEOXYGENATION OF BIO-OIL MODEL COMPOUND TO PRODUCE RENEWABLE FUEL OVER NI-BASED SUSTAINABLE CATALYSTS - (C112) 332

UPGRADING OF BIOMASS-DERIVED BIO-OIL TO GASOLINE AND DIESEL-RANGE HYDROCARBONS OVER RESOURCE - EFFICIENT SUSTAINABLE CATALYSTS VIA CATALYTIC CRACKING AND HYDRODEOXYGENATION: INNOVATION AND PROSPECTS - (C113) 334

SUSTAINABLE PRODUCTION OF BIO-BASED GRAPHITE FOR LITHIUM-ION BATTERIES - (C117) 336

ATMOSPHERIC PLASMA JET SYNTHESIS OF AG/TIO_2 PHOTOCATALYSTS FOR HYDROGEN PRODUCTION AND PHARMACEUTICAL POLLUTANT DEGRADATION - (C118) 337

INFLUENCE OF ALKALI METAL PROMOTION (K, NA, CS) ON SELECTIVITY AND PRODUCTIVITY OF CUFEZN/M-ZRO_2 CATALYSTS IN CO2 HYDROGENATION - (C119) 339

DESIGN AND SIZING OF A DEMONSTRATION PLANT FOR THE ANALYSIS OF THE SUMMER SOLAR DESORPTION PROCESS IN AN OPEN-CYCLE THERMOCHEMICAL SEASONAL STORAGE SYSTEM - (C142) 341

SULFONATED POLYSULFONE AND NANOCOMPOSITE POLYMER ELECTROLYTE MEMBRANES FOR ADVANCED POWER DEVICES - (C144) 343

THERMO-FLUID DYNAMIC ANALYSIS OF THE AIR PRE-HEATHER FOR A SOFC SYSTEM FED BY AMMONIA - (C148) 344

PRESSURISATION STRATEGIES FOR SOLID OXIDE ELECTROLYSIS CELLS: A COMPARATIVE OVERVIEW - (C156) 346

ELECTROCHEMICAL WATER OXIDATION FOR IN-ORBIT H_2O_2 PRODUCTION: TRL-4 VALIDATION IN A FLOW-CELL REACTOR - (C158) 348

ELECTROCHEMICAL WATER OXIDATION FOR IN-ORBIT H_2O_2 PRODUCTION: INSIGHTS ON MECHANISM FROM RRDE ANALYSIS - (C159) 350



MULTIFUNCTIONAL GETESE CHALCOGENIDE AS A PROMISING ELECTRODE MATERIAL FOR ADVANCED LITHIUM-ION BATTERIES - (C162) 352

MULTIPHYSICS FINITE ELEMENT MODELING OF ELECTRIFIED STRUCTURED CATALYSTS FOR SUSTAINABLE HYDROGEN PRODUCTION - (C170) 354

ENHANCED PHOTOCATALYTIC HYDROGEN PRODUCTION FROM GLYCEROL OVER G-C_3N_4 PREPARED BY SUPERCRITICAL CO_2 MICRONIZATION ROUTE - (C172) 356

SUSTAINABLE BIO-MOF-DERIVED CARBON NANOFIBROUS ELECTROCATALYSTS FOR VANADIUM REDOX FLOW BATTERIES - (C173) 358

HARMONIZED TEST PROTOCOLS AND TRAINING PROGRAMS FOR GREEN HYDROGEN PRODUCTION, STORAGE/CONVERSION AND FUEL CELL TECHNOLOGIES - (C177) 360

IONIC LIQUID-MODIFIED HYBRID POLYMERIC MATERIALS FOR THERMAL ENERGY STORAGE APPLICATIONS - (C181) 362

AN INTEGRATED EXPERIMENTAL AND MOLECULAR DYNAMICS APPROACH TO CORRELATE OXIDE-ION FRAMEWORK AND FUNCTIONAL PROPERTIES IN DOPED SRFEO3 ELECTROCATALYSTS - (C188) 363

GREEN HYDROGEN GENERATION AND BIOMASS DEGRADATION VIA A PHOSPHOMOLYBDIC ACID-MEDIATED ELECTROCHEMICAL APPROACH - (C189) 365

CATALYTIC SUPERCRITICAL WATER GASIFICATION OF WET AGRO-INDUSTRIAL RESIDUES: TAILORING RENEWABLE GAS PRODUCTION THROUGH Ni-BASED CATALYSTS - (C195) 367



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Plenary



Luigi Crema - Director of the Sustainable Energy Center at the Bruno Kessler Foundation in Trento (Italy)

Luigi Crema is the director of the Sustainable Energy Center at the Bruno Kessler Foundation in Trento. A physicist, he focuses on issues related to energy transition and the development of technological solutions linked to hydrogen and batteries. He is Vice President of the Italian Hydrogen Association (H2IT) and a board member of Hydrogen Europe Research, part of the European Clean Hydrogen JU partnership. In 2010, he received the Luigi Stringa award dedicated to "Research for Innovation."

For over twenty years, he has been involved in innovation, balancing work in both research and industrial sectors, with extensive experience in transforming development areas into practical solutions and economic value.

Among his main projects and collaborations:

- Coordination of 4 European projects: Digespo, Eden, CH2P, and Switch, in addition to participation in over 40 R&D&I projects in the energy sector, focusing on hydrogen, batteries, solar energy, and materials applied to energy.

- Author of more than 100 scientific contributions.

- Extensive support for European Commission programs, starting with FP7. Co-author of the Clean Hydrogen JU program for Horizon Europe, which he has supported since its inception in 2018, serving as the leader of Technical Committee 1 on hydrogen production.

- Active participation in numerous energy-related initiatives such as EERA, FCH JU, and CTN Energia.

- Support for the creation of spin-offs and start-ups, including Unitec in 2000 and Green Energy Storage in 2015.

- Author of 4 patents (one pending) on various topics, from the use of new materials in energy systems to safety aspects in automotive applications.

- Support to national political institutions on energy issues and involvement in several national and international initiatives.





Juergen Garche - Senior Professor at Ulm University (Germany)

Juergen Garche is Senior Professor at Ulm University, where he has held the position of Senior Professor of Electrochemistry since 2015.

He has around fifty years of experience in the fields of batteries — including lead-acid, Ni-MH, Li-ion and Na-ion systems — as well as fuel cells (PEMFC, DMFC) and electrolyzers (PEMEL).

Throughout his career, he has published 365 scientific papers, holds 10 patents, and is the author or editor of 10 books, among them the seven-volume second edition of the Encyclopedia of Electrochemical Power Sources.

He serves on the editorial boards of four journals dedicated to battery and fuel cell research and has been listed by Thomson Reuters among the "World's Most Influential Scientific Minds." He is also featured in the book Profiles of 93 Influential Electrochemists.

Professor Garche has held numerous visiting professorships at leading international institutions, including Shandong University in China, Sapienza University of Rome in Italy, TUM-CREATE in Singapore, the Dalian Institute of Chemical Physics in China, and the CNR Institute for Advanced Energy Technologies in Messina, Italy. From 1993 to 2004, he served as General Manager of the Electrochemical Energy Storage and Conversion Division at the Center of Solar Energy and Hydrogen Research (ZSW) in Ulm. Since 2004, he has been Managing Director of FCBAT (Fuel Cell and Battery Consulting) in Ulm.

He has also acted as a consultant for numerous organizations and institutions, including the German Federal Ministry of Transport, the German National Hydrogen and Fuel Cell Organization (NOW), the South African Department of Science and Technology, battery developers in several countries, and major automotive manufacturers such as BMW, Daimler, and Nissan.





Josè A. Odriozola - Professor Emeritus at the University of Seville (Spain)

José A. Odriozola, Yantze River Scholar Professor at Beijing Forestry University, is Emeritus Professor at the University of Sevilla and elected member of the Royal Academy of Sciences of Sevilla. His research work is dedicated to Catalysis and Surface Chemistry, with a focus on Sustainable Chemistry for the Circular Economy, his research primarily explores heterogeneous catalysis, particularly the study of catalyst and catalytic reactions using operando methods. Since the late 1980s, Odriozola has pioneered techniques such as operando Diffuse Reflectance Infrared Fourier Transform Spectroscopy to understand catalytic reactions and has expanded his interests to include structured catalysts and metal alloy oxidation.

He earned his Ph.D. from the University of Sevilla in 1981, focusing on the interaction of probe molecules with rare-earth oxides' surfaces. His postdoctoral research at Lawrence Berkeley Laboratory under Prof. Gabor Somorjai deepened his insights into surface chemistry, contributing to foundational work in Scanning Tunneling Microscopy.

Odriozola has authored over 400 research papers and holds 12 patent applications in catalyst design and catalytic processes. He has supervised over 40 Ph.D. students, along with numerous MSc students and Postdoctoral Research Fellows. He has been awarded with the Senior Award of the Iberoamerican Society of Catalysis in 2024. His career accolades include serving as Head of the Department of Inorganic Chemistry at the University of Sevilla, Visiting Professor of the Universities of Strasbourg, Rennes 1, Surrey and Beijing Forestry and receiving recognition as a Fellow of The Royal Society of Chemistry (FRSC) in 2022.





Alexandr N. Simonov - Associate Professor, Associate Head for Industry Engagement
School of Chemistry, Faculty of Science, Monash University (Australia)

Alexandr N. Simonov is a physical chemist specialising in electrochemistry, materials science and sustainable technologies. Research in his group is aimed at understanding and designing new effective ways to generate and use renewable electricity for the sustainable energy and chemistry technologies. His major research focuses on the development of materials, electrode architectures and practical electrolytic devices for the production of hydrogen through splitting of water, reduction of nitrogen to ammonia, as well as selective oxidation of ammonia to nitrates and nitrites. He collaborates with industry on projects aiming to develop new cost-effective water electrolysers. He is a co-founder of a spin-out company Jupiter Ionics Pty Ltd. working on the commercialisation of the Monash technologies for the renewable ammonia and fertiliser production.



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Satellite Events

GRIPHUS Project

Green Innovative Photocatalytic systems for CO_2 Utilization to produce e-fuelS

Adele Brunetti[a], Marjeta M. Maček Kržmanc[b], Eugene A. Kotomin[c], Domenico Macrì[d]

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The GRIPHUS project aims to develop an innovative pathway for the production of e-fuels through the valorisation of CO_2-rich off-gas from biogas upgrading processes. By combining advanced photocatalytic systems and membrane technologies, the project will demonstrate a new generation of integrated photocatalytic membrane reactors capable of enhancing CO_2 conversion efficiency under continuous operation.

Biogas upgrading is a well-established technology for biomethane recovery; however, the resulting CO_2 stream is still largely considered a waste product. GRIPHUS proposes a paradigm shift by transforming CO_2 into a valuable carbon feedstock for the production of green chemicals and e-fuels. In particular, captured CO_2 will be converted through hydrogenation with renewable hydrogen into key platform molecules, such as methanol, supporting the European transition towards sustainable fuels and circular carbon-based processes.

The project will deliver a robust proof of concept through the design, construction, operation and validation of a laboratory-scale advanced photocatalytic membrane reactor in a relevant environment. The approach integrates the development of innovative photocatalysts and membrane materials with complementary expertise in DFT modelling, fluid dynamics, reaction engineering and process simulation. Multiscale modelling will support the understanding and optimization of catalytic structures, reactor performance and the overall integrated process, including techno-economic assessment and life cycle analysis.

Sustainability is a key driver of GRIPHUS. The project will explore environmentally friendly preparation routes, including green solvents and biodegradable polymers for membrane fabrication. Moreover, end-of-life strategies will be investigated to recover and reuse valuable components, including polymers and photocatalysts, enabling circular approaches beyond the first application cycle.

Structured into seven interconnected work packages over three years, GRIPHUS aims to advance the integrated technology from TRL 2–3 to TRL 5, demonstrating its feasibility in a relevant operating environment. By converting CO_2 from an environmental challenge into a renewable carbon resource, GRIPHUS contributes to the development of sustainable e-fuels and to the transition towards a circular, low-carbon European economy.

GRIPHUS is an international collaborative project co-funded by the Regione Calabria, the Ministry of Higher Education, Science and Innovation of Slovenia, and the Latvian Council of Science within the framework of the M-ERA.NET Call 2024. The consortium includes four partners from Italy, Slovenia and Latvia, comprising three academic/research institutions and one industrial partner, bringing together complementary expertise in photocatalysis, membrane engineering, modelling and process development.

Acknowledgments

This project is co-funded by Regione Calabria, Ministry of Higher Education, Science and Innovation of Slovenia and Latvian Council of Science in the framework of M-Era.Net call 2024

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RISEnergy – Project

Research Infrastructure Services for Renewable Energy

Research Infrastructure Services for Renewable Energy (RISEnergy) project is dedicated to fostering a long-term, coordinated research effort among leading private companies and research institutions to advance energy technologies within the EU. RISEnergy targets the EU's Horizon Europe Framework Programme topic focused on "Research infrastructure services to enable R&I addressing main challenges and EU priorities,'' specifically addressing the sub-topic "RI services for renewable energy technologies and systems. In this regard, RISEnergy aims to integrate services provided through a network of energy-related research infrastructures (RIs) in both the EU and Associated Countries, namely in the fields of Photovoltaics (PV), Concentrated Solar Power (CSP)/ Solar Thermal Electricity (STE), Hydrogen, Biofuels, Wind Energy, Ocean Energy, Integrated Grids, Energy Storage, Material Science and Information and Communication Technology (ICT). https://risenergy-project.eu/

RISEnergy Session 1: Research Infrastructure networks in Europe: best practices, challenges and barriers: the experience of the RISEnergy ecosystem.

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Keywords: research; infrastructure; best practices, ecosystem, data

Abstract: The acceleration of the clean energy transition is central to the EU's industrial strategy, energy security, and competitiveness. In this context, the RISEnergy project establishes a coordinated European ecosystem of Research Infrastructures (RIs) to support innovation in renewable energy technologies and system integration.

One of the key ambitions of RISEnergy is to accelerate Europe's clean energy transformation, through systematic support to collaborative innovation, a necessary element for EU competitiveness. Within the RISEnergy ecosystem, 80+ RIs play a core role by providing access to their facilities, physically and remotely. Most of these RIs also belong to the ecosystem of the European Energy Research Alliance (EERA), that ensures synergies all over the R&I energy landscape across Europe.



This session will discuss results and ongoing challenges from RISEnergy's Work Package 1, aimed at ensuring that this ecosystem efficiently works and exchanges with all the other activities and external initiatives, delivering transversal results for the project's achievement. In particular, it identifies technology and research gaps that can improve access, interoperability and exploitation of research outputs.

WP1 also gathers best practices from the research infrastructures networks involved in the project, assessing national and transnational external access (TA/VA/EA) to energy Research Infrastructures.

All these efforts serve as drivers to strengthen EU competitiveness, a more structured share of public funding, and eventually a stronger research ecosystem, with positive spillovers for EU industrial value chains as well.

As the role of data becomes increasingly central for RIs, the session will also deal with the results on data and metadata procuration and standardization, currently analysed in WP3 of RISEnergy, as a key challenge for RI access sustainability.

Acknowledgements

This session was supported by the RISEnergy project. The project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101131793.

RISEnergy Session 2: From Idea to Impact: How RISEnergy Research Infrastructures and Services Foster Innovation

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Keywords: research, infrastructure, innovation, access, transnational

Abstract: Europe is at a critical stage in its energy transition. Achieving climate neutrality while ensuring energy security, system resilience, and global competitiveness requires faster, smarter, and more collaborative research and innovation pathways. Research infrastructures (RIs) play a central role in this process, yet their potential remains insufficiently exploited.

This session introduces the RISEnergy project, which coordinates an ecosystem of more than 80 world class research infrastructures dedicated to renewable energy. Through its Transnational Access and Innovation Services, RISEnergy supports both research driven and innovation oriented activities by providing access to advanced experimental facilities, specialised expertise, digital tools, and testing environments covering a wide range of renewable energy technologies and systems. User experiences demonstrate how access to RISEnergy infrastructures accelerates research progress, strengthens methodological robustness, and supports the transition from research concepts to innovation ready solutions.

The session provides practical insights into accessing RISEnergy services and discusses how artificial intelligence and system integration approaches—including within the framework of the RISEnergy ESFRI proposal—can further enhance research impact and collaboration between academia and industry.



Objectives of the session:

- Showcase the role of European research infrastructures in advancing smart and sustainable energy technologies
- Present RISEnergy Transnational Access and Innovation Services as a practical pathway from research to application
- Explain how potential users can access, test, and validate technologies within the RISEnergy ecosystem
- Share concrete results and lessons learned from RISEnergy user experiences
- Discuss how digital tools, AI, and system integration approaches can further enhance innovation outcomes (RISEnergy ESFRI proposal)

Acknowledgements

This session was supported by the RISEnergy project. The project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101131793.

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IAGE- Italy - Round Table

IAGE Italy
INTERNATIONAL ASSOCIATION FOR GREEN ENERGY

The International Association for Green Energy is a non-profit organization that builds an educational and informative platform for networking and knowledge exchange across academia, industry, and society at large in all areas of green energy.

It promotes the creation of an Italian scientific network aimed at fostering scientific development in the fields of renewable energy and sustainable energy production processes, whilst also striving to protect the environment and improve quality of life. It represents the Italian branch of the association's international division.

As part of ICSET 2026, the Italian branch of the International Association for Green Energy (IAGE) will organize a round table bringing together representatives from academia, research institutions, industry, and public stakeholders to discuss current challenges, emerging opportunities, and future perspectives in green energy technologies and sustainable energy systems

Challenges and Perspectives of Green Energy in the Next Decade

Round Table organised by IAGE-Italy at ICSET 2026

Adolfo Iulianelli*

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Keywords: green energy; energy transition; renewable energy; green hydrogen; sustainable energy systems; research-industry collaboration

Abstract: The International Association for Green Energy (IAGE) is a not-for-profit organization that provides an educational and information platform for networking and knowledge exchange among academia, research bodies, industry and society across all areas of green energy. Its Italian branch, IAGE-Italy, promotes a national scientific network devoted to renewable energy, sustainable energy production processes, environmental protection and improved quality of life, while contributing to the wider international activities of the Association.

Within ICSET 2026, IAGE-Italy will organize the round table "Challenges and perspectives of green energy in the next decade". The session will bring together recognized experts from universities, research institutions and international scientific networks to examine the technological, industrial and societal conditions needed to accelerate the transition towards secure, competitive and low-carbon energy systems. Discussion will cover the integration of variable renewable sources, energy storage and grid flexibility, green hydrogen and sustainable fuels, efficiency and circularity, industrial decarbonization, infrastructure and supply-chain development, together with the regulatory, financial and skills-related barriers that may affect deployment.



By combining perspectives from Italy, Türkiye and the Czech Republic, and expertise spanning hydrogen strategies, catalytic and chemical processes, integrated energy systems, materials, environmental technologies and applied research, the round table will move beyond individual technologies and consider the energy system as a whole. The exchange is expected to identify shared research and innovation priorities, highlight demonstration and scale-up needs, and outline concrete opportunities for cross-sector and international cooperation in the decade ahead.

Invited speakers

Dr. Luigi CREMA - President of Hydrogen Europe Research and Director of the FBK Center for Sustainable Energy

Prof. Vincenzo PALMA - Full Professor at the University of Salerno and Vice-President of IAGE-Italy

Prof. Ozgur C. COLPAN - Full Professor at Dokuz Eylul University and President of IAGE-Türkiye

Dr. Leonarda LIOTTA - Research Director at the National Research Council of Italy

Dr. Jan VERES - Researcher at VSB-Technical University of Ostrava and incoming President of IAGE-Czech Republic

Dr. Gianluca LANDI - Senior Researcher at the National Research Council of Italy and Member of IAGE-Italy

Moderator

Dr. Adolfo IULIANELLI, Senior Researcher at the National Research Council of Italy and President of IAGE-Italy



RdS 25-27- Special Sessions

- **Electrochemical and Thermal Storage Technologies**
- **Ammonia as a Hydrogen Carrier in the Energy Transition**

RdS
RICERCA DI SISTEMA

The Ricerca di Sistema (RdS) is the instrument by which MASE finances research activity for innovation in the Italian energy sector. CNR, ENEA and RSE represent the three research groups financed by the MASE to carry out projects considered strategic for the growth of our country.

Special session - Electrochemical and Thermal Storage Technologies:

The new integrated project "Electrochemical and thermal storage technologies" is structured to cover the different segments of the storage systems value chain, in continuity with the previous three-year implementation plan (PTR). This project proposes experimental activities along two main lines, both of which are essential to contribute to achieving the objectives set by the new National Integrated Plan for Energy and Climate (PNIEC) by 2030. Many activities look at more innovative or cutting-edge storage solutions, capable of contributing in the medium-long term to the growing energy needs resulting from the large-scale integration of non-programmable renewable sources. These new technologies must guarantee not only adequate performance in terms of capacity and duration (compared to consolidated technologies), but also a reduced environmental impact, in line with the principles of sustainability and decarbonization. The project consists of 5 work packages (WP) within which the different Activity Lines (LA) are outlined. WP1 is dedicated to the development of materials for electrochemical storage. The activities focus on the synthesis and characterization of innovative electrode materials and electrolytes for batteries at various stages of technological development. Special attention is given to improving the performance, safety, and sustainability of established technologies (Li-ion gen.3 and 4) and innovative technologies (Li-metal, Na-ion, and flow batteries). It is important to note that a major development effort, undertaken by the entire project team, focuses on Na-ion technology, which is considered one of the most promising and strategically important for our country. The goal is to optimize assembly procedures and treatments and to identify a common path that will lead to the development of a complete Na-ion cell within the project. Significant research efforts are directed toward exploring frontier technologies (metal-air, anodeless battery). WP2 is dedicated to the development of advanced tools for the diagnostics, monitoring, and control of electrochemical storage systems. These tools will combine data-driven models, supported by artificial intelligence, with physical and chemical models. The primary objective is to estimate the State of Health (SoH) and the Residual Useful Life (RUL) of batteries by conducting laboratory tests on Li-ion cells and other technologies, such as Na-ion. The activities will involve sharing aging data for cells through common databases, which were developed and made public in the previous PTR, and will be updated with new datasets. WP3 focuses on cross-cutting activities that span the different technologies, materials, and systems explored in WP1 and WP2. The main activities include Life Cycle Assessment (LCA) and Life Cycle Inventory (LCI) studies, which are dedicated to evaluating the production of materials developed in WP1 and in the previous PTR. WP4 focuses on the development of efficient and sustainable thermal storage systems. The key challenges include the use of high-energy density materials to reduce volume, the creation of durable and cyclable materials to enhance stability and lifespan, the design of systems that can quickly adapt to varying charge/discharge rates, and the reduction of costs with environmentally friendly solutions. WP5 is dedicated to the management and internal communication of the project, as well as the dissemination of results and stakeholder engagement through the organization of events, seminars, and workshops. The primary goal of the project is to serve as a catalyst for the development and innovation of storage materials and technologies, with a strong emphasis on enhancing performance, safety, and sustainability. Through its integrated approach and the synergy between the different sectors involved, the project will act as a driving force to accelerate the development of technologies capable of meeting the demands of a rapidly evolving global market.



Special session - Ammonia as a Hydrogen Carrier in the Energy Transition

The integrated project on Hydrogen Technologies and End Uses (RdS PTR 2025–2027, Theme 1.3), coordinated by ENEA and carried out jointly with CNR, RSE and a broad consortium of Italian universities, proposes a vast and articulated research programme addressing multiple technologies along the entire hydrogen value chain from production to storage, transport and final uses. The project focuses on innovative solutions at medium-to-low technological maturity (TRL 3–5), in line with the decarbonisation, energy security and research competitiveness objectives of the Italian National Integrated Plan for Energy and Climate (PNIEC). Within this framework, ammonia occupies a strategic position across multiple work packages. In WP1, dedicated to sustainable hydrogen production, the project investigates innovative pathways alternative to conventional electrolysis, including photoelectrocatalytic water splitting, thermochemical processes and the conversion of renewable or recycled carbonaceous feedstocks such as biogas always in a circular economy perspective and with systematic coupling to concentrated solar thermal and photovoltaic energy sources. WP2 focuses on the storage and transport of hydrogen, with ammonia identified as one of the most promising hydrogen carriers alongside liquid organic hydrogen carriers (LOHCs). Research activities target the development of new materials and processes for large-scale hydrogen storage in the form of ammonia, its safe handling, and the integration of power-to-gas and power-to-fuel conversion routes. In parallel, catalytic hydrogenation processes and the reconversion of existing industrial infrastructure including refineries and natural gas networks are explored to support the transition towards a green hydrogen economy. WP3 addresses the end uses of hydrogen and its carriers, with particular attention to ammonia in electricity generation and hard-to-abate sectors. Key activities include the development of flexible combustion systems for microturbines powered by methane/hydrogen and ammonia/hydrogen mixtures, advanced MILD (Moderate and Intense Low-oxygen Dilution) combustion technologies for ammonia/hydrogen fuels, and a thorough analysis of the explosive behaviour of such mixtures to ensure safe deployment at scale. Innovative fuel cell systems and the exploitation of methanol in port applications complete the end-use portfolio. Taken together, the activities of Theme 1.3 contribute to building a robust national hydrogen and ammonia supply chain, reducing dependence on fossil fuels, and enabling the decarbonisation of sectors where direct electrification remains technically or economically unfeasible.

The results presented in this session reflect research advances achieved within the 2025–2027 programme and discuss prospects for further scale-up and industrial integration.

This special session explores the strategic role of ammonia as a carbon-free hydrogen carrier in the ongoing energy transition. Bringing together researchers and experts from National and European projects, the session covers the full ammonia-to-hydrogen chain from green synthesis and catalytic cracking to reactor design and end-use applications in power generation and hard-to-abate sectors. Opening with the presentation of the Italian RdS 2025–2027 research programme, the session offers a focused forum to discuss recent technical advances, share results, and identify synergies for a sustainable hydrogen-ammonia economy.



Abstracts

Plenary

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HIGH SUSTAINABILITY AND ENVIRONMENTAL REQUIREMENTS FOR BATTERIES AND BATTERY SAFETY - (P001)

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Keywords: Sustainable Energy, Renewable Energies, Environment, Batteries, Battery Safety

1. Introduction

The global energy sector is undergoing a strong transformation (energy transition, Energiewende). The share of renewable energies in electricity generation is steadily increasing (2025: 34.3%), while in other sectors such as heating (2025: 12.5%) and fuels (2025: 4%), the share of renewables is significantly lower. The transmission leads to a sharp increase in battery demand, especially due to:

A - The high share of volatile renewables (solar, wind) of currently > 70% requires dispatchable power capacity (gas, hydro, H2/FCs, batteries, etc.) to compensate for periods of low renewable energy production, with the share of batteries growing rapidly.

B - In the transport sector batteries play an increasingly important role in replacing fossil fuels. While EVs currently only account for 4% of the total vehicle fleet, the new registration rate is around 25%.

The demand for batteries is growing exponentially (2 TWh in 2025, estimated at 7…10 TWh in 2030). This leads to enormous challenges in battery production, use, and disposal.

2. Requirements for battery production, use and end-of-life

Life Cycle Thinking (LCT) principles based on sustainability (safety, environmental, social, and economicy) are to applied for:

- *Raw material extraction*: Sustainable and ethical sourcing (co-mining in the Congo, child labor), reduction of critical materials, minimization of environmental impact (water consumption)
- *Production*: Energy-efficient manufacturing, emissions and waste reduction, renewable energies use
- *Use:* Batteries designed for intensive use, high specific energy, high energy efficiency, long lifespan, low degradation, and high safety.
- *End-of-life:* Second life and recycling.
- *Geopolitics:* China's LIB share: 75 %.



Figure 1: Sustainability sectors.

3. Requirements for battery safety

In the EU Safe-and-Sustainable-by-Design (SSbD) concept [1] safety refers to hazardous substances (health, environment) and hazardous substance combinations that lead to safety events (fire, explosions) in products (e.g. batteries).

Besides this pre-market SSbD approach, the battery safety topic focuses on field hazards and their causes, as well as preventive measures [2, 3] which will be the focus of the presentation.

In practice accidents with LIBs are extremely rare, in the < 0.1 ppm range. Accidents mainly occur when the cells are operated outside the operating window defined by the manufacturer. But even for these cases, a whole range of features have been developed to further increase the safety of the batteries:



Materials - using materials and material combinations with high thermal stability and low combustion energies. When selecting materials, it must be considered the temperature at which the cathode material decomposed under release of oxygen which reacts with the organic electrolyte and the anode and leads to fire and explosions (thermal runaway).

Engineering - via cell design and electrical and mechanical safety features.
E.g. the ratio of cell volume (proportional to cell energy) to the cell surface (proportional to cooling performance), burst discs and their arrangement in the cell as well as pressure and temperature sensors and other safety features as protection circuit boards (PCB), positive temperature coefficient resistors (PTC), circuit interrupt devices (CID) and battery management systems (BMS).

A particular challenge is posed by the increasing specific cell energy (max. semi-ASSB: 600 Wh kg^{-1}) and their capacity (LFP – max. 2,710 Ah), which leads to an enormous increase in cell energy. Such developments are only possible through consistent, safety-relevant improvements to the cell material and design.
A further challenge is the increasing energy of battery applications (max. BESS Abu Dabi: 19 GWh) which is only possible by preventing thermal propagation from a failed cell to neighboring cells. Finally, the safety of Na-ion and ASSB technologies will be discussed in relation to Li-ion systems.

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TANDEM CATALYSIS: ONE-POT SAF SYNTHESIS FROM CO_2 – (P002)

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Keywords: One-pot SAF synthesis, Tandem Catalysts, Fe-based Fischer-Tropsch catalyst, Machine Learning.

1. Introduction

FTS is a chemical process that converts syngas into hydrocarbons mainly focusing on liquid fuels. The success of the FTS has been traditionally linked to oil prices although the circular economy scenario has prompted a renewed interest in FTS since the use of unconventional carbon sources for biofuel production. However, supply, energy management, processing, chemistry, and engineering are challenges that results in biofuels significantly more expensive than conventional fuels. Nevertheless, process intensification could lead to more competitive biofuels but demanding the use of a new generation of nanoengineered catalysts capable of maximizing selectivity towards a specific product, achieving maximum feedstock conversion, ensuring high robustness, and excellent durability.[1]

Tandem catalysis, a subcategory of one-pot reactions, combines multiple reactions within a single reactor. The concept of one-pot synthesis is addressed to integrate appropriate synthetic and catalytic steps into a unified process, thereby transforming a reagent into a final product. Tandem catalysis of readily available substrates, such as carbon dioxide, into valuable products represents an effective approach to reducing the cost and environmental impact of chemical processes.[2] Selective tandem catalyst for FTS requires different types of catalytic sites and to strictly follow a reaction sequence. Designing tandem catalysts for synfuels must consider the desired fuel, the suitable Fischer-Tropsch active phase, the upgrading phase, the agreement between operating conditions, the catalyst shape, and the catalyst cost. Here we highlight the advances and challenges in harnessing unconventional feedstocks and integrating renewable energy using the synthesis of SAF from CO_2 as an example.

2. Materials and Methods

A comprehensive set of analytical tools allowed conventional, in situ and operando techniques for catalyst characterization among them HAADF -STEM coupled EDX; In situ and *Operando* DRIFTS and NAPXPS. Machine learning was used for modelling conversion and selectivity responses. T, P, GHSV and TOS were used as predictors; targets included single-pass conversions and carbon-based selectivities.

Catalytic activity measurements were conducted in a fixed-bed reactor. Gas fraction was analysed online by GC and liquid fraction offline by GC-MS and GC with FID. Carbon balances are always better than 85 %.

3. Results and Discussion

The integration of FTS with HCR, presents a promising strategy to enhance the efficiency and selectivity of chemical reactions crucial for liquid fuel production. Yet, this integration also surfaces optimization challenges, notably in balancing the maximization of liquid fuel yield against maintaining process simplicity and compactness.

However, the transition to practical applications highlights several challenges, including CO_2-conversion efficiency, catalyst poisoning in raw syngas scenarios, feed gas composition's impact on product distribution, and the durability of catalytic phases



under operational conditions. Furthermore, the complexity of these new systems necessitates deriving insights from intricate and deep relationships that may not be discernible through traditional optimization and enhancement mechanisms. In this paradigm, leveraging cutting-edge AI tools could represent a turning point for the optimization, design, and fine-tuning of new catalysts. Integrating these advanced strategies will undoubtedly be crucial in the future of biofuels using tandem catalysts.

All these concepts are demonstrated using Fe-base catalysts for SAF production. These catalysts yielded a broad, olefin-rich product distribution, requiring further catalytic upgrading to produce SAF. The best Fe-based catalyst alone produces ~60 wt.% linear olefins and <5 wt.% cyclics, a product distribution that differs from SAFs standards. A secondary function is added by physically mixing the Fe catalyst with ZSM-5 zeolite forming a tandem catalyst that enriches middle distillates (C_6-C_{16}). Machine-learning-assisted interpolation enabled the identification of optimal operational windows for maximizing conversion and C_5^+ selectivity on Fe-ZSM-5 tandem catalyst, table 1.

Table 1. Conversion and selectivity of the optimized tandem catalyst.

Feedstock	$WHSV$	Conversion (%)	Selectivity	
			CH_4	C_{5+}
CO_2	7 L g^{-1} h^{-1}	39.4	4.9	72.7
CO	2 L g^{-1} h^{-1}	93.9	3.3	51.3

4. Conclusions

Promising conditions for jet fuel production were identified, we leveraged high-pressure *operando* DRIFTS to observe the Fe catalyst surface during the CO_2-to-hydrocarbons reaction. The study revealed intermediate species consistent with Fischer-Tropsch synthesis as well as methanol-to-hydrocarbon reactions. The results highlighted the importance of reducing the Bronsted acidity and incorporating hydrogenating activity in the catalyst to produce more saturated, linear products needed for jet fuel.

Acknowledgements

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REDOX-MEDIATED ELECTROSYNTHESIS OF AMMONIA FROM RENEWABLES - (P003)

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Keywords: electrolysis, NRR, hydrogen, oxygen evolution reaction

1. Introduction

Over several years of research, the lithium redox-mediated nitrogen reduction reaction (Li-NRR) has evolved from an essentially forgotten, low-productivity process into one of the most technologically promising methods for the conversion of dinitrogen to ammonia. This was supported by the demonstration of Li-NRR at the ammonia yield rates above 1 μmol s^{-1} cm^{-2}, current-to-ammonia (faradaic) efficiencies close to 100%, and electrolytic devices coupling the Li-NRR and the hydrogen oxidation reaction (HOR) for ammonia electrosynthesis from N_2 and H_2 on a timescale of weeks. Notwithstanding this progress, the Li-NRR systems are still facing a range of critical limitations preventing its translation into industrial applications, even at a small scale. The most prominent challenges that are yet to be addressed include: (i) instability of the Li-NRR cathodes at practical current densities, (ii) poisoning and degradation of the HOR anodes under the Li-NRR conditions, (iii) fundamental limitations of coupling the Li-NRR with the most technologically desirable anode process, *viz.* the oxygen evolution reaction (OER), and (iv) low energy efficiency, which is inherently limited by the redox potential of the $Li^{0/+}$ mediator.

2. Results and Discussion

In our group, we investigate and develop strategies that might help to address the limitations above. This includes advances in water electrolysis for the production of sustainable hydrogen, which is required for the operation of the Li–NRR|HOR electrolysers. At the Li-NRR cathode level, we use advanced methods, including *in situ* spectroelectrochemical techniques, to understand the evolution and degradation mechanisms of the key system components in operation. This understanding guides the development of new, more robust Li-NRR electrolytes and electrodes. At the device level, we develop the Li-NRR|HOR devices operating at elevated pressure, as opposed to the state-of-the-art operation at ~1 atm, as well as of the Li-NRR|OER cells that avoid an interference between the organic N_2 reduction and aqueous O_2 evolution electrolyte media. Finally, we explore new materials that can enhance the energy efficiency of the Li-NRR by enabling N_2 reduction at potentials more positive than the reversible $Li^{0/+}$ potential. The lecture will present some of the major outcomes of our work in this area.

Acknowledgements

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SHUNT, PARASITIC AND REVERSE CURRENTS IN BIPOLAR ELECTRODE STACKS – (C001)

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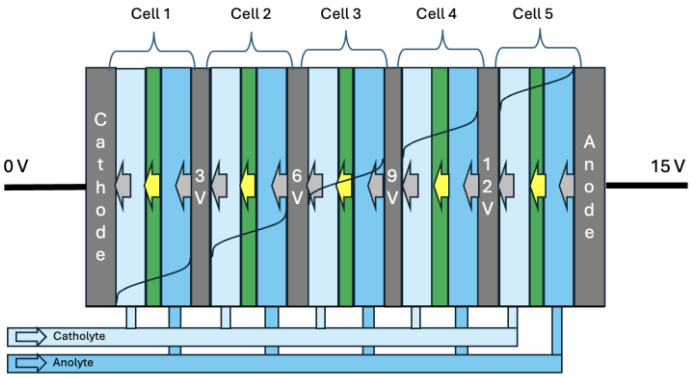
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Keywords: water electrolysis, bipolar electrodes, stack

1. Review

Large-scale water electrolysis is considered one of the major stepping-stones of the energy transition, enabling the production of green hydrogen and paving the way for green ammonia, green steel, and sustainable aviation fuels (SAFs). Although gigawatt-scale electrolysis capacity is being planned, most installations today fall in the 10–100 MW range, well below the current European ambitions.

In this lecture, we will discuss shunt currents, parasitic currents, reverse currents, and degradation mechanisms in bipolar electrode stacks when water electrolysis systems are interfaced with intermittent energy sources. In particular, we will examine the inherent challenges associated with operating alkaline or PEM electrolyzers at low loads.



Parallel electrodes separated by electrolyte solutions in the presence of a membrane (green). Grey arrows represent redox currents; yellow arrows represent ionic currents through the ion-permeable membranes and in the electrolyte solutions.

2. Conclusions

Operating an electrolyzer stack at low loads is challenging as it is difficult the potential distribution between each electrode pairs.

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SYNTHESIS AND CHARACTERIZATION OF PELLETIZED PEROVSKITES FOR GREEN HYDROGEN PRODUCTION BY TWO-STEP THERMOCHEMICAL WATER SPLITTING CYCLE – (C006)

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Keywords: Hydrogen, CSP, Thermo-chemical Cycles, Solar Fuel, Perovskites

1. Introduction

Perovskite oxides are promising redox materials for two-step thermochemical water splitting due to their tunable oxygen non-stoichiometry.

Thermal reduction $$ABO_3 \rightarrow ABO_{3-\delta} + \frac{\delta}{2} O_2$$

Water shift $$ABO_{3-\delta} + \delta H_2O \rightarrow ABO_3 + \delta H_2$$

This study examines the feasibility of operating both the reduction and the steam-oxidation steps at temperatures not exceeding 1000 °C in a fixed-bed reactor (FBR) system. Two different pelletization methods were investigated to obtain pellets with suitable size and performance for this type of application, using perovskites synthesized from non-toxic precursors. By comparing the results, the most effective method was selected and applied to the tested perovskite materials in the FBR. Overall, it was possible to detect hydrogen during steam oxidation by gas chromatography, thus enabling the calculation of hydrogen yields.

2. Materials and Methods

In this work, the perovskite powders used for pelletization were selected with an emphasis on sustainable materials to support green hydrogen production. The pellets were characterized by XRD, SEM, and BET analyses, and their thermal stability was evaluated by TGA. Qualitative analysis of the gas produced during the thermochemical cycle was carried out using a custom fixed-bed reactor system. The gaseous products were analyzed with a Varian 4900 microGC connected to the reactor outlet.

3. Results and Discussion

$Ca_{0.8}Sr_{0.2}MnO_3$ (CSM821) powder was selected for pelletization for its good redox capabilities. Two methods were investigated, and the results are summarized in Table1:

- **Polyvinyl alcohol (PVA) method** – By optimizing the solid-to-liquid (S/L) ratio and adding γ-Al_2O_3 as an inert support, the PVA pelletization method produced pellets with good mechanical strength, porosity, and structural stability. XRD, SEM, and TGA analyses confirmed a good redox performance under thermal cycling comparable to that of the powder.
- **Dough method** – The pellets obtained are mechanically stronger but non-porous; moreover, the bentonite support alters the perovskite structure, reducing redox capabilities. Thermal stability is maintained after the initial water loss.



Table1. Results comparison between the two pelletization methods.

Synthesis Method	Support Material	δ_{fin} [-]	Stability	Mechanical Resistance	Scalability of pelletization method
PVA (20°C/min; S/L = 36.7 %wt)	-	0,214	Good	Low	Hard
PVA (20°C/min; S/L = 36.7 %wt)	γ Al_2O_3 (20 %wt)	0,191	Good	Low	
PVA (2°C/min; S/L = 36.7 %wt)	γ Al_2O_3 (50 %wt)	0,202	Good	Very Low	
PVA (2°C/min; S/L = 73.4 %wt)	-	0,182	Very Good	Medium	
Dough	Bentonite (50 %wt)	0,0213	Good	Very Good	Easy

The amount of H_2 produced in HP-TGA during the hydrolysis step is below the detection limit of the laboratory instrument (<10 ppm). Consequently, as shown in Figure 1, a quantitative test was carried out using 2.5 g of CSM821 pellets, i.e., a sample mass about two orders of magnitude higher than the TGA capacity. GC analysis confirmed the presence of H_2 in the outlet gas.

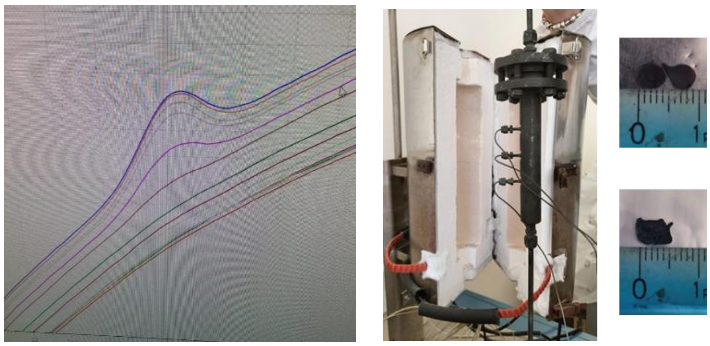


Figure1. On the left, H_2 peak detected by GC. In the center, the fixed-bed reactor used for the experimental campaign. On the right, CSM821 pellet size obtained with the PVA method (top) and the dough method (bottom).

4. Conclusions

This study compares two pelletization methods, highlighting their strengths and drawbacks. The PVA method proved to be the most suitable for FBR applications, offering a good compromise between mechanical robustness and redox performance. Data collected in the FBR system are more representative than TGA measurements, demonstrating the feasibility of a perovskite-based two-step thermochemical water-splitting cycle operating below 1000 °C. This approach offers a potential pathway toward more energy-efficient redox hydrogen production.

Acknowledgements

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ACTIVITY-STRUCTURE DEPENDANCE ON SURFACE CRYSTAL PHASE OF ALLOY Pd-Cu NANOPARTICLES FOR THE HYDROGEN OXIDATION REACTION – (C008)

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Keywords: Anion exchange membrane fuel cells; Hydrogen oxidation catalyst, PdCu alloy.

1. Introduction

The alkaline hydrogen oxidation reaction (HOR) is a fundamental anodic reaction in anion exchange membrane fuel cells (AEMFC). State-of-the-art catalysts require high loadings of PGM group metals such as Pt-Ru and Pd-CeO_2.[1] Pd-Cu alloy nanoparticles with appropriate surface crystal phases can be tuned by thermal treatments to afford enhanced alkaline HOR activity through optimized hydrogen binding energy (HBE) and a favourable OH_{ad} binding energy (OHBE). Here we report the controlled synthesis of a Pd-Cu alloy by vapor phase synthesis with a 1 to 1 atomic ratio (Pd_1Cu_1). Post synthetic treatment at 500 °C under inert atmosphere transforms the PdCu alloy surface from FCC to a mix FCC-BCC phase leading to an increase in HOR activity of more than one order of magnitude.

2. Materials and Methods

Using a standardized Metal Vapor Synthesis (MVS) procedure, palladium and copper vapors are generated by resistive heating of two different alumina-coated tungsten crucibles filled with Pd (150 mg, powder) and Cu (50 mg, beads). They were co-condensed simultaneously at liquid nitrogen temperature with acetone (100 mL) in a glass reactor. The resulting PdCu NPs were then supported on carbon (metals 10 wt%) and heat treated at 500 °C under flowing N_2.

3. Results and Discussion

The controlled synthesis of the Pd-Cu alloy was achieved by vapor phase synthesis with a 1 to 1 atomic ratio (PdCu). Post synthetic treatment at 500 °C transformed the PdCu alloy surface from FCC to a mix of FCC-BCC phases. Electrochemical measurements show that this change leads to an increase in HOR activity of approximately one order of magnitude (I_0 9.2 vs 1.5 A g^{-1}). The anode catalysts (PdCu and 500°C-PdCu) were incorporated into MEAs for testing in AEMFCs with an electrode surface area of 5 cm^2. Fuel cell tests showed higher power densities for 500°C-PdCu (peak power densities 0.9 vs 0.8 W cm^{-2}) and the heat-treated catalyst was more stable over longer testing including stop-start cycles.

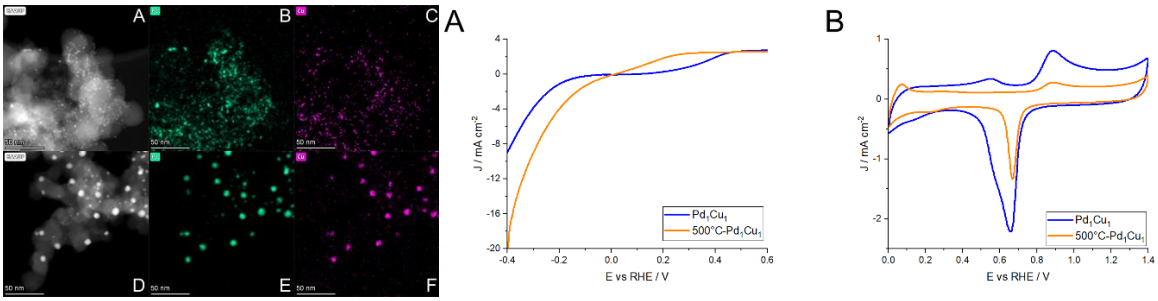


Figure 1. STEM-EDX micrographs of (A-C) PdCu and (D-F) 500°C-PdCu. (A) LSV acquired in H_2 saturated 0.1 M KOH solution at 1mV s^{-1} and 1600 rpm and (B) CV acquired in N_2 purged 0.1 M KOH solution at 20 mV s^{-1}.



4. Conclusions

A metal vapor synthesis (MVS) procedure was used to prepare PdCu nanoparticles with a 1:1 atomic ratio. Heat treatment at 500 °C transformed the surface crystal phase from BCC to a mix BCC-FCC. Such a surface has a combination of optimized hydrogen binding energy and a favourable OH_{ad} binding energy. The increase in activity after heat treatment translates directly to higher power densities in AEMFC testing.

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OPERANDO DRIFT INVESTIGATION OF CU-BASED CATALYSTS DURING CO_2 CONVERSION TO METHANOL IN PRESENCE OF GREEN HYDROGEN – (C009)

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Keywords: Operando DRIFT Spectroscopy; methanol; green hydrogen; CO_2 conversion; Cu catalysts.

1. Introduction

By looking at the recent advances on CO_2 hydrogenation for the production of methanol (MeOH), numerous studies have focused on the activity and adsorption properties of copper-based catalysts [1,2], often leveraging on forced structure-activity relationships to propose plausible mechanisms governing the reaction path, so that the nature of the active sites therein involved and the intermediates regulating the process remain subjects of ongoing debate. It is well known that in the CuO–ZnO–ZrO_2 (CZZ) catalytic system, the redox state of copper plays a fundamental role both in H_2 activation and in the establishment of a suitable metal-oxide interface as crucial to promote CO_2 activation and the subsequent formation of intermediates leading to MeOH production [3]. Therefore, to disclose the specific functionality and lifetime of surface species involved in the reaction pathway, operando techniques, such as Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) coupled with Mass Spectrometry (MS), can effectively enable real-time monitoring of intermediate species under relevant experimental conditions, aiming to provide crucial insights for the optimization of MeOH catalysts.

2. Materials and Methods

A previously optimized CZZ catalyst with a composition of 60/30/10 at/at was synthesized via gel–oxalate coprecipitation to evaluate its activity-selectivity-stability pattern during methanol synthesis via CO_2 hydrogenation. The reaction was carried out in a fixed-bed reactor in the temperature range of 180–260 °C at a pressure of 3.0 MPa ($CO_2/H_2/N_2$, 23/69/8 v/v), the catalyst being characterized both before and after each run to assess any possible physico-chemical modification. To monitor the formation of surface species involved in the key steps of the process, parallel *operando* DRIFTS-MS measurements were performed in an environmental chamber located inside a *Nicolet iS50 (ThermoFisher Scientific, USA)* spectrometer directly coupled with a *HPR-20* (*Hiden Analytical, UK*) quadrupole mass spectrometer, as a real-time detector of gaseous products.

3. Results and Discussion

The catalytic system was investigated upon activation under different atmosphere (H_2 or CO/He reduction at 0.1 MPa and 300 °C for 1 h against no pre-reduction). No significant differences in catalytic performance were observed with respect to the activation protocol, this result clearly suggesting that, due to the large volume of H_2, the reaction mixture is able to directly generate *in situ* the active sites required for MeOH formation, making the initial pretreatment step largely irrelevant.

Interestingly, operando measurements revealed a competition between the two claimed reaction pathways for MeOH synthesis as function of the adopted conditions. As shown in Figure 1, at a temperature as low as 180 °C, formate species predominate, whereas above 220 °C the Reverse Water–Gas Shift (RWGS) reaction becomes prominent, with a prevalence of carbonate and bicarbonate species and CO as a reaction intermediate. With no pre-reduction step, the formate pathway does not seem to take place at low temperature, although the formation of MeOH at 180 °C. This highlights the reducing capability of the reaction mixture with time on stream, underscoring the critical role of the Cu^0/Cu^+ pair in both H_2 activation and stabilization of intermediate species.



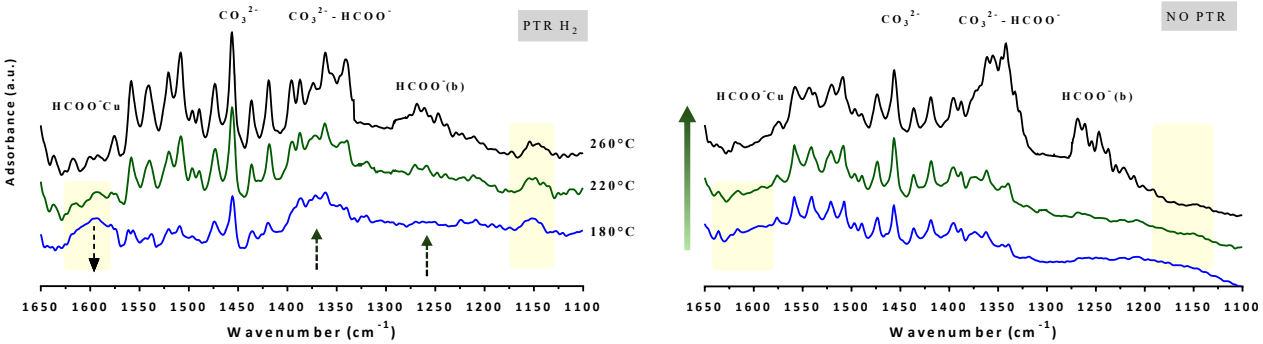


Figure 1.IR spectra acquired on C6Z1Z3 after H_2 pre-reduction (left) and with no pre-reduction (right) during the CO_2 hydrogenation reaction at 3.0 MPa in the temperature range 180-260 °C.

4. Conclusions

CuO–ZnO–ZrO_2 formulation is effective in driving the formation of MeOH via CO_2 hydrogenation, the specific atomic composition significantly influencing the formation of active sites and intermediates. Due to the reducing capability of the reaction mixture, the sites necessary for the hydrogenation of CO_2 to MeOH are generated upon the process, suggesting the possibility to avoid the step of catalyst pre-activation. From a mechanistic point of view, *operando* DRIFT investigations indicate that operating conditions and chemical environment play a key role in modulating the reaction pathways, since at low temperature MeOH formation mainly proceeds via formate intermediate, whereas at higher temperature the CO formation becomes prominent via RWGS.

Acknowledgements

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EFFECT OF CONVENIENTLY FUNCTIONALIZED NANOMATERIALS ON ANION EXCHANGE MEMBRANES FOR WATER ELECTROLYSIS – (C010)

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Keywords: Anion Exchange Membranes, nanocomposite membranes, PFG-NMR, ionic conductivity, alkaline water electrolysis.

1. Introduction

Anion exchange membranes for water electrolysis (AEMWE) are a promising route to sustainable hydrogen production, as they enable the use of low-cost, non-precious metal catalysts in alkaline enviroment. However, achieving a balanced combination of high hydroxide conductivity, efficient water transport and robust chemical durability remains the main challenge [1]. Among the strategies proposed to address these issues, nanofillers incorporation has shown significant potential [2]. In this work, nanocomposite AEMs were prepared by introducing variously functionalized carbon dots (CDs), a new class of carbon nanoparticles, into quaternary ammonium-functionalized polysulfone (qPSU) to study the effects of fillers on membrane's structure, transport properties and electrochemical performace.

2. Materials and Methods

Membranes' morphology, physicochemical properties and electrochemical performance were investigated. NMR spectroscopy provided insight into molecular dynamics through the direct measurements of the self-diffusion coefficients using PFG-NMR and spin–lattice relaxation times (T_1), while EIS was used to assess ionic conductivity. Finally, membrane performance was assessed in a single-cell water electrolyzer to check the effect of CDs on the cell performance.

3. Results and Discussion

The incorporation of CDs in qPSU membranes influences their properties. The effectiveness of the filler is dictated by its functionalization (Fig. 1) which influences the polymer–filler interactions, a key factor in determining membrane properties. Nanocomposite membranes generally exhibited different morphology and physicochemical properties in comparison with pristine which indicate changes in hydrophilicity and ionic site accessibility, directly connected to water uptake and ion exchange capacity. NMR investigations revealed that nanofillers affect molecular dynamics and water retention capacity at high temperatures. Electrochemical impedance spectroscopy confirmed significant changes in hydroxide conductivity for nanocomposites. Across all investigated systems, it has been found that quaternary ammonium-functionalized carbon dots effectively optimized membrane morphology, water dynamics and ion transport. Furthermore, these improvements ensured superior water electrolysis performance, sustaining higher current densities than qPSU and making them highly promising nanofillers for high-performance and durable AEMs.



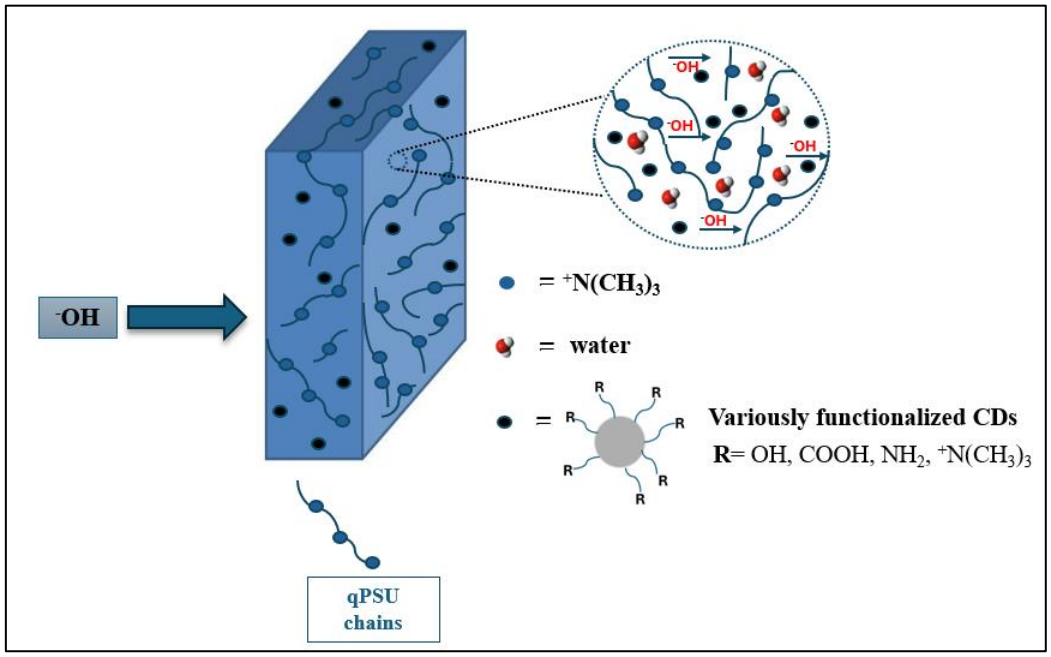


Figure 1. Schematic rapresentation of qPSU+CDs membrane.

4. Conclusions

Overall, the results demonstrate that functionalized nanofillers work as integral components of polymeric membrane, enabling simultaneous changes in structure, water dynamics, conductivity and electrochemical performance for anion exchange membrane water electrolysis.

Acknowledgements

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SUSTAINABLE HYDROGEN UPGRADING FROM SYNGAS THROUGH ULTRA-MICROPOROUS CARBON HOLLOW FIBER MEMBRANES – (C011)

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Keywords: carbon hollow fibre membranes; gas separation; H_2 purity and recovery; syngas upgrading

1. Introduction

Biomass gasification is a mature technology that is increasingly considered economically viable and competitive with conventional natural gas reforming. The process converts carbon-containing materials into synthesis gas, mainly composed of H_2, CO, CO_2, CH_4, H_2O, and N_2, with compositions depending on feedstock and process conditions. Membrane gas separation is an attractive option for H_2 purification due to high recovery, simple operation, and energy efficiency. Among membrane materials, carbon-based membranes—particularly hollow fibre types—offer high permeability, selectivity, and chemical stability under high temperatures and pressures. This study investigates green-based ultra-microporous carbon membranes for H_2 upgrading from syngas. Experimental investigation analysed the permeation of binary and ternary gas mixtures of various compositions and at different temperatures. Permeation data were the input of the process simulations to investigate membrane configurations for H_2 upgrading from syngas.

2. Materials and Methods

The hollow fibres were spun from a P84 polyimide dope using the green solvent γ-butyrolactone, thereby avoiding conventional dipolar aprotic solvents. Together with a simple water-based post-treatment and N_2 carbonization, this approach reduces solvent hazards compared to traditional routes while yielding ultra-microporous carbon fibres with high selectivity. Their separation performance was examined using binary and ternary gas mixtures over a range of feed compositions and temperatures. The results were used as inputs for a model implemented in Python and in DWSIM.

3. Results and Discussion

In this study, we demonstrated the potential of polyimide-derived carbon hollow fibre membranes, fabricated via a sustainable spinning process using green solvents and subsequent controlled carbonisation, for efficient H_2 separation from binary and ternary gas mixtures. The membranes exhibited a heterogeneous ultramicroporous structure, as confirmed by excellent Sips isotherm fitting, underpinning their high selectivity and operational robustness. Mixed-gas permeation measures showed consistently superior H_2 permeance, which increased with its molar fraction in the feed. CO_2 displayed moderate permeance governed by competitive sorption, whereas CO had the lowest permeance, particularly at higher feed concentrations. Analysing the results obtained from the separation of a ternary mixture at 80°C with a composition of H_2:CO:CO_2 = 29.9:29.4:40.7 reveals that the hollow fibre carbon-based membranes presented in this study confirm a preferential selectivity towards H_2 and lesser for CO_2. Examining the permeate composition, it is clear that these membranes significantly enhance the concentration of H_2, increasing it to 57% in the permeate. At the same time, the CO fraction is significantly reduced to 4%, corresponding to an 87% decrease compared to the initial value (Figure 1). Process simulations allowed to design a multistage membrane process able to maximize the recovery of a H_2 rich stream. A single-stage system showed an intrinsic purity/recovery trade-off, whereas with a two-stage design about 86% of the hydrogen contained in the syngas was recovered with a concentration of 90% (Figure 2).



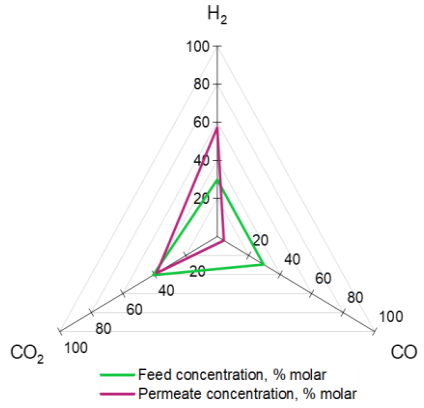


Figure 1. Feed and permeate composition for a ternary mixture H_2:CO:CO_2 = 29.9:29.4:40.7 at 80°C

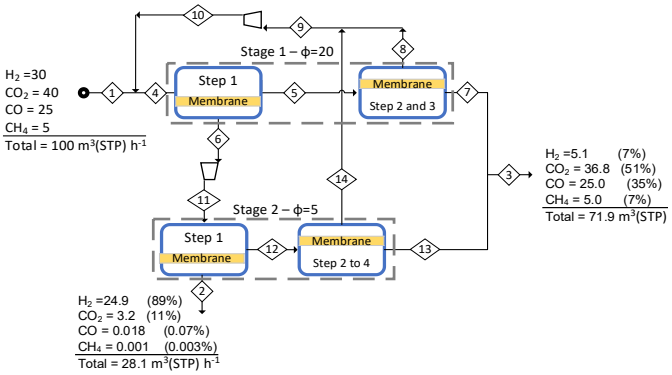


Figure 2. Multi-stage membrane process for syngas upgrading.

4. Conclusions

This study demonstrates polyimide-derived carbon hollow fibre membranes fabricated via sustainable spinning with green solvents and controlled carbonisation for efficient H_2 separation from binary and ternary mixtures. A heterogeneous ultramicroporous structure, supported by Sips isotherm fitting, enabled high selectivity and robustness. A two-stage process achieved 90 mol% H_2 purity at 86% recovery, highlighting strong potential for H_2 purification, CO_2 capture and gas separation.

Acknowledgements

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ELECTRIFIED SORPTION-ENHANCED CATALYTIC DRY REFORMING OF METHANE FOR CLEAN HYDROGEN PRODUCTION – (C012)

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Keywords: methane dry reforming, joule heating, structured conductive catalysts, calcium looping, carbon capture.

1. Introduction

Driven by climate change and decarbonization goals, hydrogen has emerged as a promising energy carrier, and methane dry reforming ($CH_4+CO_2 \leftrightarrows 2CO+2H_2$; $\Delta H°=247$ kJ/mol) represents a viable production route through the simultaneous conversion of two greenhouse gases. To mitigate CO_2 emissions associated with the high heat demand of this endothermic process, electrified reactors based on Joule heating offer an attractive approach with potential economic and environmental benefits [1]. To achieve net-zero CO_2 emissions downstream, calcium looping (CaL) can be integrated into the process within carbon capture and storage (CCS) frameworks [2]. In this context, the TIPIC project (*"Innovative technologies for the production of clean H_2 without CO_2 emissions"*) aims to address this challenge by developing electrified catalytic reactors integrated with sorbents for clean hydrogen production.

2. Materials and Methods

The structured Ni/CeO_2-Al_2O_3 catalyst was prepared starting from a SiSiC foam, used as the carrier due to its high thermal conductivity. A γ-alumina-based washcoat was applied via dip-coating, while ceria as support and nickel as the active phase were introduced through wet impregnation technique. The experimental setup includes a Joule-heated electrified reactor and a mass spectrometer to monitor outlet stream composition. Calcium oxide granules were used as solid sorbent to assess CO_2 adsorption capacity and sorbent selectivity.

3. Results and Discussion

Nitrogen physisorption at 77 K and mercury intrusion porosimetry confirmed the micro- and mesoporous structure of the catalyst, while SEM-EDX analysis highlighted the homogeneous dispersion of the Al_2O_3 washcoat on the SiSiC carrier surface, as well as of ceria and nickel oxide. Temperature-programmed reduction (TPR) analysis confirmed good reducibility properties, which can be attributed to the uniform dispersion of the catalytic phase.

Preliminary reaction tests were carried out in a Joule-heated electrified reactor at different space velocities using a feed composition of 45% v/v CO_2, 45% v/v CH_4 and 10% v/v Ar. At a WHSV of approximately 22 h^{-1}, a hydrogen yield of 73% was achieved. The process exhibited an energy consumption of 2.47 kWh/m^3H_2, lower than the value (2.6 kWh/m^3H_2) currently reported in the literature [3] at comparable WHSV, and an energy efficiency (ε) of about 91% (ε=TEC/EEC*100) was reached at a temperature of approximately 800°C (Fig.1a). In parallel, with a view to the final objective, CO_2 carbonation–calcination cycles on calcium oxide ($CaO+CO_2 \leftrightarrows CaCO_3$) were conducted. Initial findings indicate that, over successive cycles, the sorbent exhibits a progressive decrease in its adsorption capacity (Fig.1b). In particular, starting from the 10th cycle, the adsorption capacity decreases more markedly, while beyond the 15th cycle the curve tends to level off, suggesting the presence of a residual capacity of the material. This behavior can be attributed to the loss of available surface area, as confirmed by BET analysis performed on spent calcium oxide compared to the fresh material, indicating the occurrence of sintering effects, in agreement with literature reports [2]. Early observations were obtained from additional tests carried out to investigate the sorbent behavior toward the other components present in the outlet stream of a dry reforming catalytic stage. The results show that no desorption peaks were observed for the individual compounds in the binary mixtures (Ar–CH_4, Ar–CO, Ar–H_2) or in the overall simulated gas mixture representing the dry reforming outlet stream, in which only CO_2 adsorption and desorption peaks were detected. These findings confirm the absence of competition with the other components, indicating that the adsorption energies of CO, CH_4, and H_2 on CaO are very low and have a negligible impact on CO_2 adsorption.



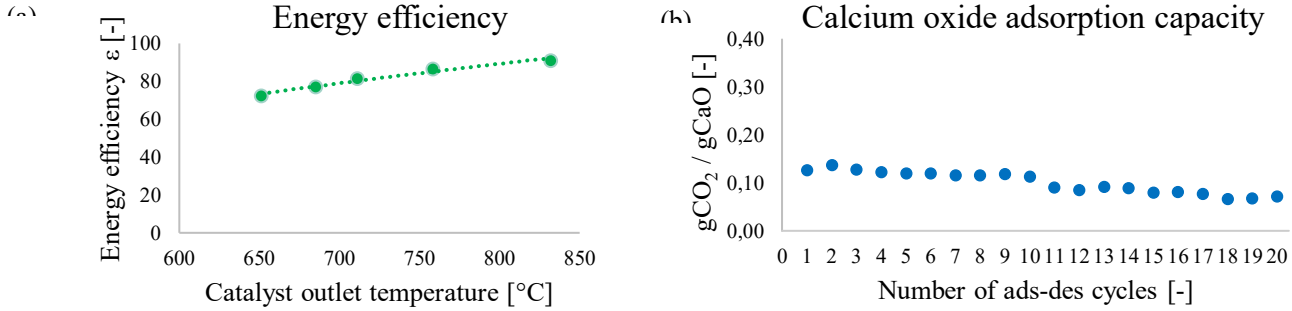


Figure 1. (a) Process energy efficiency as a function of catalyst outlet temperature at WHSV = 22 h^{-1}; (b) Sorbent capacity ($gCO_2/gCaO$) as a function of the number of carbonation–calcination cycles.

4. Conclusions

The experimental results confirm the potentiality of this process, particularly due to the low experimental energy consumption (2.47 kWh/m^3H_2), which is below the value reported in the literature (2.6 kWh/m^3H_2) for comparable WHSV, and the high energy efficiency achieved (91.47%). An updated literature review highlighted the possibility of further improving performance by adding a second metal to the catalytic formulation to mitigate potential coking and sintering. Future developments will also include preheating the reactant mixture during dry reforming to improve the thermal profile and optimize heat transfer, thereby enabling the design of an optimal system for the future integration of CO_2 capture sorbents.

Acknowledgements

This project has received funds from the project "Tecnologie innovative per la produzione di H_2 clean senza emissioni di CO_2-TIPIC" - Id. domanda RSH2A_000036, funded by the MASE - funded within the National Recovery and Resilience Plan (NRRP), Mission 2, Component 2, Investment 3.5.

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FROM CO_2 TO POWER: ASSESSING THE ENVIRONMENTAL IMPACTS OF POTASSIUM FORMATE AS CHEMICAL ENERGY CARRIER – (C014)

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Keywords: Life cycle assessment (LCA), Electrolyzer, Direct Formate Fuel Cell (DFFC), Potassium Formate (PF), CO_2-to-Power

1. Introduction

The EU Horizon project FRESH (Formate for Renewable Energy Storage) offers an innovative solution for the electrochemical conversion of captured CO_2 from various sources into a carbon-based building block, potassium formate (PF). While promising, this technology is at a low Technology Readiness Level (TRL) but has significant potential for development. This energy carrier produced by renewable electricity and captured CO_2, integrating the carbon capture and utilization (CCU) principle, is used in next-generation fuel cell technology to provide on-demand, electrical power.

2. Materials and Methods

This study presents a Life Cycle Assessment (LCA) of PF production via a co-electrolyzer, and its reconversion to electricity using new direct formate fuel cell (DFFC) technology. In a cradle-to-gate approach, the study evaluates the environmental impacts related to this FRESH-concept using CO_2 sources from direct air capture, biomass and cement plants as carbon source. Based on experimental data from the project and a techno-economic assessment (TEA) main drivers for various environmental impacts are identified.

3. Results and Discussion

The results show that the investigated environmental impacts are all dominated by the operation phase. The high amounts of KOH needed for the operation of the DFFC contribute between 41 and 49% to almost all environmental impacts. The rest stems mainly from the production of PF, where again the needed KOH solution is main reason for the impacts. The base-case, using CO_2 captured from a cement plant has the highest impacts in the group of CO_2 sources. Overall, the impact of the different CO_2 sources on all environmental impact categories is relatively small.



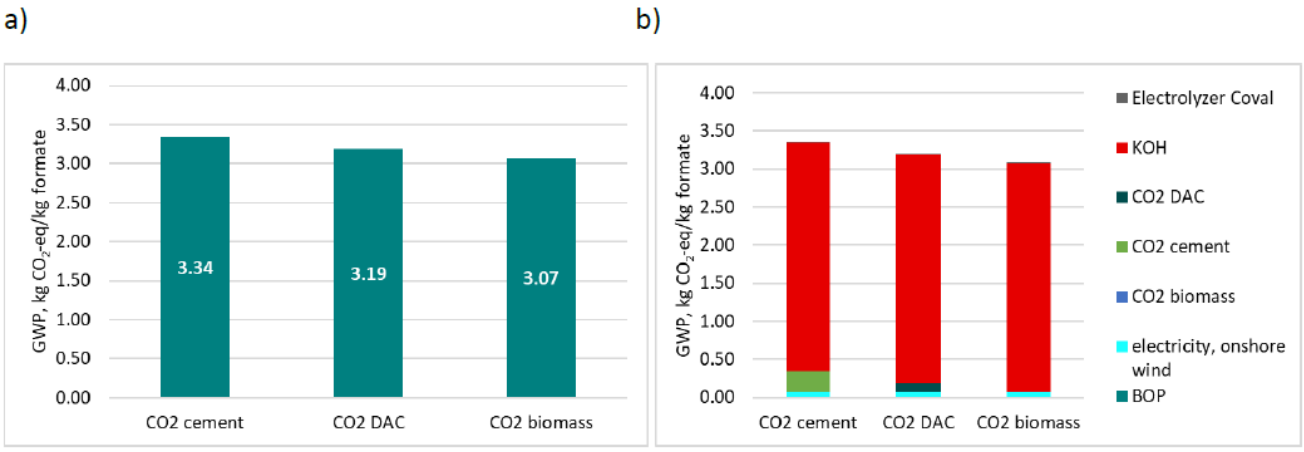


Figure 1. *GWP associated with the production of 1 kg of PF from various sources of CO_2; a) absolute GWP per kg of PF, b) absolute contribution per component and process in GWP per kg of PF.*

4. Conclusions

The environmental impacts from the FRESH-concept when re-generating electricity from stored PF produced via co-electrolysis were investigated in an LCA. Climate change impact is mostly induced by the use of KOH. But also other environmental impacts are dominated by it. This study suggests that reduction or recycling of KOH must be the main emphasis for further research.

Acknowledgements

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SO-FREE: FROM SYSTEM ARCHITECTURE TO COMMISSIONING OF A MULTI-FUEL SOFC PLATFORM – (C015)

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Keywords: Multi-fuel, SOFC-CHP, System integration & commissioning.

1. Introduction

Solid oxide fuel cells (SOFCs) enable high-efficiency CHP, making them attractive for industrial decarbonization. However, real deployment is slowed by the need to operate across variable fuels (H2/NG/biogas) while respecting tight stack constraints, managing reforming/steam balance, and meeting safety and certification requirements; most platforms remain tuned to a single fuel and stack supplier. SO-FREE aims to deliver an industrial SOFC system architecture that is truly multi-fuel and stack-agnostic, with automatic adaptation during fuel switching. Novel elements include anode off-gas recirculation to provide process steam and a methane-bypass control concept, now implemented in a fully integrated test rig.

2. Materials and Methods

An industrial SOFC-CHP test rig was designed and built including fuel conditioning/reforming, anode off-gas recirculation, heat management and power electronics. A supervisory controller plus independent SIS/ESD handle start-up/purge and automatic switching among H2/NG/biogas. Component sizing was supported by partner simulations (mass/energy, transients). During commissioning tests, T, P, flows and gas composition are logged to evaluate stability and switching performance.

3. Results and Discussion

Commissioning of the fully integrated SO-FREE test rig has started, focusing on functional checks, heat-up, purge/safe-state validation, and closed-loop operation under controlled fuel supply. First steady-state runs on hydrogen confirm stable stack conditions and a net electrical efficiency of ~50% (LHV basis), in line with expectations for SOFC-CHP at the selected operating point. Early power maps indicate that the supervisory controller can maintain controlled operation while varying inlet fuel, providing a practical basis to extend testing to methane/biogas and mixed-fuel operation.

Over the next months (project end: June), the test campaign will generate a structured dataset covering fuel switching, transient response, thermal balance, and endurance. The discussion will therefore focus on defining the validation metrics and the evidence pathway: (i) repeatable start-up/shutdown and safe-state transitions, (ii) power/efficiency versus fuel composition, (iii) stability of key constraints (temperature/gradients, fuel utilization proxies, and boundary conditions at the stack interface), and (iv) robustness against realistic disturbances (fuel quality and load changes).



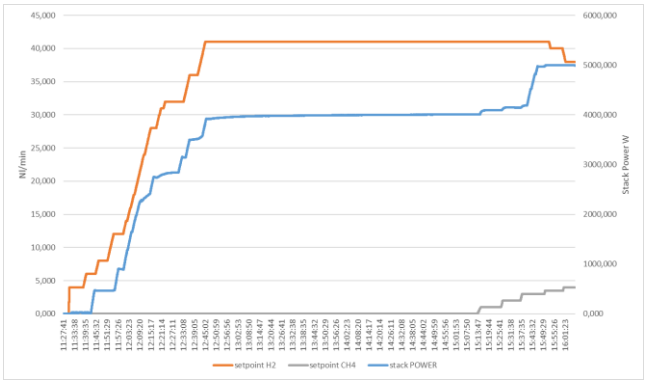




Figure 1. Net electrical power as a function of inlet fuel composition (H2/NG/biogas blend) during initial commissioning tests (photo of the integrated rig shown separately).

4. Conclusions

SO-FREE demonstrates an industrial integration approach for SOFC-CHP systems targeting true fuel flexibility and stack-agnostic interfaces. The integrated rig has entered commissioning; first hydrogen runs show stable operation and ~50% net electrical efficiency (LHV). By June, planned tests will quantify switching, transients and endurance, supporting replication of the approach for decarbonized CHP and H2-ready industrial applications.

Acknowledgements

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Ni EXSOLUTION AND DEFECT CHEMISTRY OF La(Sr)Mn(Ni,Cr)O_3 FOR SOFC AND SOEC ELECTRODES – (C016)

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Keywords: Perovskite oxide, exsolution, SOFC, SOEC

1. Introduction

Exsolution is a beneficial process that promotes the uniform growth of highly dispersed catalytically active nanoparticles partially embedded in surface sockets of the host oxide, enhancing their stability. Perovskite oxides (ABO_3) are widely favored as host materials due to their remarkable structural flexibility, allowing for various element substitutions and controlled crystal defect chemistry, which are crucial for manipulating the exsolution process. They also possess tunable ionic and electronic conductivity and can be designed to maintain stability under redox conditions and high temperatures, making them highly suitable for energy conversion applications like fuel cells and electrolyzers. Nickel is one of the most effective exsolvable species for such systems, owing to its high reducibility, favorable incorporation as a B-site dopant, and excellent catalytic activity. The in-situ formation of Ni nanoparticles enhances not only the electrochemical activity of perovskite-based electrodes but also provides a cost-effective alternative to noble metals. [1,2]

2. Materials and Methods

In this study, we investigate Ni exsolution from La(Mn,Cr)O_3-based perovskites with controlled A-site doping and defectivity using Sr. Ni-doped La(Mn,Cr)O_3 powders were synthesized by Solution Combustion Synthesis. All obtained materials were characterized by X-ray diffraction (XRD) combined with Rietveld refinement, scanning electron microscopy (SEM), thermogravimetric analysis (TGA) and electrical conductivity measurements under controlled pO_2. Sample powders were reduced using 5%H_2

3. Results and Discussion

Thermogravimetric analysis performed under reducing conditions showed clear differences in mass loss behavior among the investigated compositions, which can be attributed to variations in oxygen vacancy formation and the onset of Ni exsolution. These results point to a strong dependence of the reducibility of the perovskite lattice on the dopant concentration and A-site defectivity. Consistently, electrical conductivity measurements are used to elucidate the role of A-site doping in modulating the transport properties of the materials, leading to improved conductivity for selected compositions.

SEM analysis of the reduced samples confirmed the formation of Ni nanoparticles exsolved at the perovskite surface, with a high degree of dispersion. The particle size and surface density were found to be closely related to the A-site chemistry, the overall defect structure of the host lattice and the exsolution condition. Taken together, these findings indicate a clear link between compositional tuning, exsolution dynamics, and the resulting microstructural and functional properties, supporting the suitability of these materials as durable and efficient fuel electrodes for SOFC and SOEC applications. [3]



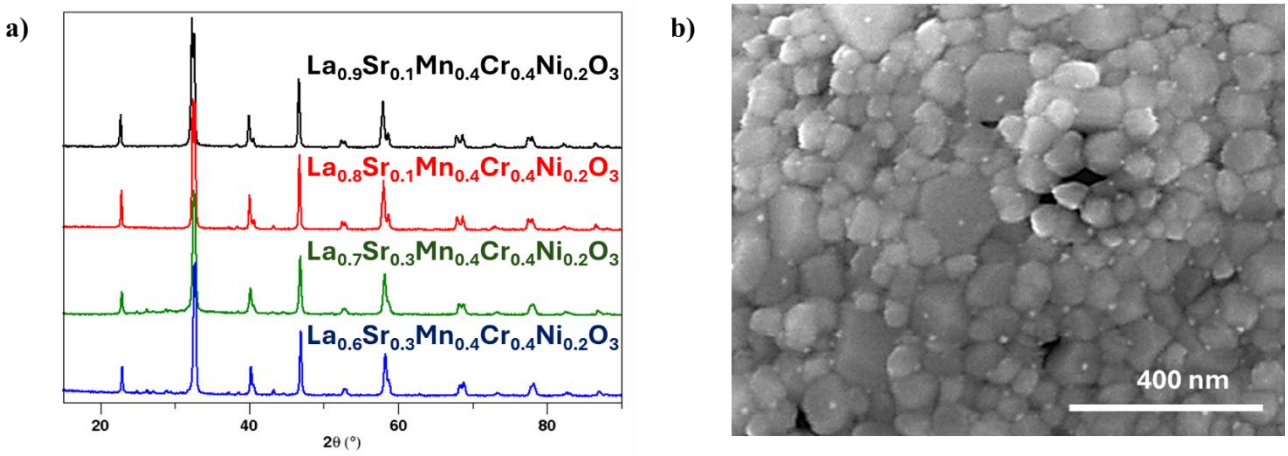


Figure 1: a) XRD pattern of non-exsolved samples; b): SEM micrograph of the reduced $La_{0.8}Sr_{0.1}Mn_{0.4}Cr_{0.4}Ni_{0.2}O_3$ composition, showing exsolved Ni nanoparticles.

4. Conclusions

The final goal of this investigation is to establish structure-property relations across the twelve-composition series, using different amounts of dopants to modulate the exsolution process, influence the microstructural evolution of the perovskite, and ultimately impact the electrochemical properties relevant to SOFC and SOEC operation. We then elucidated the crystal chemistry, defect chemistry and microstructure of La(Mn,Cr)O_3-based perovskites. By correlating the role of A-site chemistry, and Ni content, with nanoparticle formation and stability, this work contributes to the rational design of exsolution-based fuel electrode materials with improved performance and long-term durability

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HIGH-ENTROPY OXIDES WITH SACRIFICIAL HIGH-VALENCE METALS TO OBTAIN EFFICIENT AND STABLE ELECTROCATALYSTS FOR WATER OXIDATION IN AEM ELECTROLYZERS – (C018)

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Keywords: high-entropy oxides, alkaline water oxidation, lattice-oxygen mechanism, sacrificial high-valence elements, green hydrogen production.

1. Introduction

Anion exchange membrane water electrolysis (AEMWE) combines the advantages of both alkaline water electrolysis (AWE) and proton exchange membrane water electrolysis (PEMWE), enabling the production of high-purity H_2 via the use of non-precious electrocatalysts (ECs). Nonetheless, it has not yet reached the necessary level of maturity needed for its broad market penetration [1]. This contribution focuses on the preparation and testing of an inexpensive, highly efficient and durable EC for the oxygen evolution reaction (OER). The EC, based on the high-entropy concept and containing sacrificial high-valence metals to facilitate *in-situ* surface restructuring during activation [2], is developed in the framework of the project "DURALYS" (*DURAble, Scalable, and Recyclable Components and Cell Designs for Next Generation Alkaline Exchange Membrane Water Electrolysis*).

2. Materials and Methods

A high-entropy oxide (HEOs) containing non-precious metals, some of which a sacrificial role, was prepared via the synthesis route described in a previous paper [3] and characterized by several analytical techniques. Its electrochemical behavior was evaluated in 1 M KOH solution within a 5 cm^2 zero-gap AEMWE cell by recording linear sweep voltammetry (LSV) curves at different temperatures in the 30–80 °C range. The membrane-electrode assembly (MEA) consisted of the HEO-based anode, a PiperION® membrane and a conventional 40% Pt/C cathode. Chronopotentiometry was used to evaluate the EC stability.

3. Results and Discussion

The results of transmission electron microscopy (TEM), X-ray diffraction (XRD) and micro-Raman spectroscopy (MRS) analyses evidence that the pristine HEO consists of aggregates of very small grains of oxide (< 10 nm) with spinel primary phase. At 2.2 V potential, the HEO||PiperION®||Pt/C cell delivers a current density of 1.73 and 5.54 A cm^{-2} at 30 and 80 °C, respectively (Figure 1). The latter value exceeds those reported so far for precious metal-free ECs. The cell is able to stably deliver 1 A cm^{-2} for 300 h at 1.9V. *Ex-situ* analyses on the reacted EC confirm the nearly total removal of the sacrificial metals, which enables the deep pre-catalyst surface restructuring upon activation at pre-OER potential, responsible for the EC high efficiency and stability.



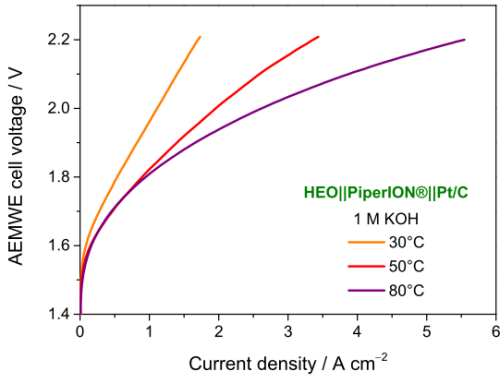


Figure 1. LSV curves recorded at different temperatures in the 30–80 °C range. HEO and Pt loads at the anode and cathode were 4.0 and 0.2 mg cm^{-2}, respectively.

4. Conclusions

The incorporation of sacrificial components into the HEO-based pre-catalyst, upon activation, leads to the formation of an extremely active and stable OER EC, which allows the AEMWE cell operating in 1M KOH to achieve a current density value never before reported for precious metal-free ECs. This work proposes a viable strategy to improve the efficiency of water electrolyzers for hydrogen production and provides new insights for the exploration of advanced OER electrocatalysts based on multicomponent materials.

Acknowledgements

The Authors gratefully acknowledge the Italian Ministries of Foreign Affairs and International Cooperation (MAECI) and of University and Research (MUR) for the financial support to this study through of Project "DURALYS, *DURAble, Scalable, and Recyclable Components and Cell Designs for Next Generation Alkaline Exchange Membrane Water Electrolysis*".

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TAILORING ANODIZED WO_3 NANOSTRUCTURES FOR PHOTOELECTROLYSIS OF BIOMASS CONTAINING SOLUTIONS AND PHOTOCATALYTIC AIR PURIFICATION – (C019)

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Keywords: biomass valorisation, H_2 production, photoelectrocatalysis, WO_3 nanostructures, Pt-free electrodes

1. Introduction

Sustainable and low-impact technologies are increasingly required to address energy and environmental challenges. In this context, anodization represents a green, low-temperature, and scalable electrochemical process for producing nanostructured oxide semiconductors with controlled properties. Anodic oxides based on valve metals are particularly attractive for photo(electro)catalytic applications due to their stability, large surface area, and easy integration into reactor-scale systems [1]. Photocatalysis and photoelectrocatalysis can harness solar energy for pollutant abatement and for coupling hydrogen production with biomass valorisation, improving both energetic and economic sustainability [2]. Tungsten trioxide (WO_3), thanks to its visible-light activity, offers a promising alternative to TiO_2 [3]. Here, anodized WO_3 nanostructures are tailored for dual application in photoelectrochemical biomass oxidation and photocatalytic air purification.

2. Materials and Methods

WO_3 nanostructures were fabricated by direct anodization at 30V of tungsten foils, followed by annealing at 500°C tailoring morphology and optical properties. Structural and morphological characterization was performed by scanning electron microscopy (SEM) and Raman spectroscopy. To get insight into the optical properties, photoelectrochemical measurements were carried out under monochromatic irradiation. Photoelectrocatalytic tests were conducted using glycerol as a model biomass-derived compound to produce glyceraldehyde (GA) and dihydroxyacetone (DHA) as high value added compound, while photocatalytic activity for air purification was evaluated using 2-propanol as a representative volatile organic compound.

3. Results and Discussion

Anodization of tungsten led to the formation of homogeneous porous WO_3 layers, in contrast to the flat oxide obtained by simple thermal oxidation. SEM analysis revealed a highly porous morphology, providing a significantly increased surface area. Raman spectroscopy confirmed the formation of monoclinic WO_3 for both flat and anodized samples. Photoelectrochemical characterization showed that WO_3 electrodes exhibit n-type behavior, with a strong photoresponse in the UV region and detectable activity extending into the visible range. The optical band gap, estimated from photocurrent spectroscopy, was ~2.9 eV, consistent with literature values. Band alignment analysis indicated that photogenerated holes possess sufficient oxidizing power to promote both direct oxidation reactions and the formation of reactive oxygen species.

In photoelectrochemical glycerol oxidation, WO_3 photoanodes enabled simultaneous hydrogen production and selective formation of value-added products. Faradaic efficiencies up to ~40% toward glyceraldehyde and ~25% toward dihydroxyacetone were achieved (Figure 1a-b), with hydrogen Faradaic efficiency approaching 100%, despite the use of an undivided cell.

To address WO_3 stability in aqueous media, photocatalytic air purification was investigated under spray-phase conditions. Porous WO_3 layers exhibited effective 2-propanol abatement, with conversions up to ~35% and formation of acetone (Figure 1c), highlighting the versatility of anodized WO_3 for sustainable environmental remediation.



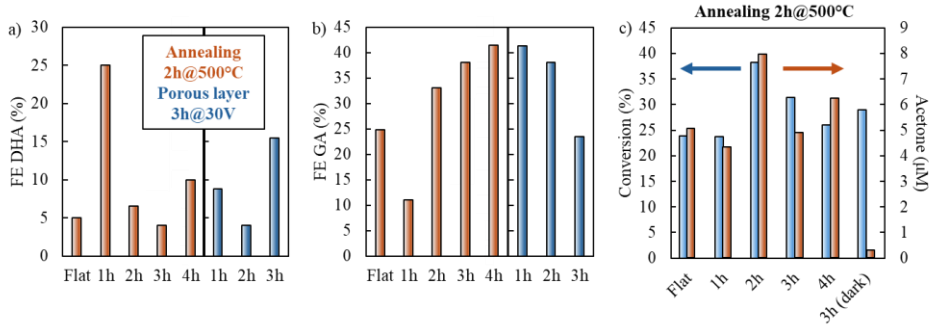


Figure 1. a) DHA and b) GA Faradaic efficiencies obtained during glycerol photoelectrolysis; c) photocatalytic performance for 2-propanol abatement in the gas (spray) phase using samples anodized or annealed for different durations.

4. Conclusions

Anodized WO_3 nanostructures were successfully tailored through a green and scalable electrochemical process, yielding photoelectrodes with tunable morphology and optical properties. The optimized WO_3 layers enabled efficient, PGM-free hydrogen production coupled with selective biomass oxidation, as well as effective photocatalytic VOC abatement. These results highlight anodization as a sustainable strategy for developing multifunctional photo(electro)catalysts for energy and environmental applications.

Acknowledgements

This work was supported by the MICS (Made in Italy – Circular and Sustainable) Extended Partnership and received funding from the European Union Next-GenerationEU (Piano Nazionale di Ripresa e Resilienza (PNRR) – Missione 4, Componente 2, Investimento 1.3 – D.D. 1551.11-10-2022, PE00000004).

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STABILITY ENHANCEMENT IN METHANOL-TO-DME CATALYTIC MEMBRANE CONTACTORS ENABLED BY BILAYER ZSM-5 MEMBRANES - (C020)

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Keywords: catalytic membrane reactor, methanol dehydration, dimethyl ether, ZSM-5 membrane, long-term stability

1. Introduction

DME is a promising clean fuel and energy carrier produced via MeOH dehydration over acidic catalysts. Water formed during the reaction inhibits acid sites, causing deactivation. Catalytic membrane contactors have shown enhanced performance by promoting water removal during MeOH dehydration[1]. However, conventional single-layer zeolite membranes suffer from an intrinsic trade-off between acidity and hydrophobicity, leading to water-induced deactivation[2]. In this work, we demonstrate the long-term stability of catalytic membrane contactors for MeOH-to-DME conversion by using thin bilayer ZSM-5 membranes with different Si/Al ratios. The architecture of the membranes and their appropriate operation enhance MeOH conversion while significantly increasing long-term stability.

2. Materials and Methods

Catalytic performance of the bilayer membranes was evaluated in a through-flow membrane reactor operating as a contactor for the dehydration of MeOH to DME. Measurements were carried out at 200–280 °C under atmospheric pressure, evaluating methanol conversion, DME selectivity and productivity. Long-term stability tests up to 300 h on stream were performed to assess water-induced deactivation.

3. Results and Discussion

The catalytic performance of bilayer ZSM-5 membranes was evaluated in methanol dehydration to DME under through-flow membrane contactor conditions. All tested configurations exhibited complete selectivity toward DME over the investigated temperature range. A strong dependence of catalytic stability on layer sequence was observed. The configuration, which combines a hydrophobic high-Si/Al layer with an underlying acidic low-Si/Al layer, showed the most stable behaviour, maintaining nearly constant methanol conversion for 300 hours on stream. In contrast, conventional single-layer ZSM-5 membranes underwent rapid deactivation, losing more than 80% of their initial activity under identical operating conditions. The reverse bilayer arrangement displayed higher initial conversion but faster deactivation, highlighting the importance of layer ordering in controlling long-term performance. Overall, the results demonstrate that an appropriate distribution of functional layers in catalytic membrane contactors effectively limits water-induced deactivation while preserving sustained catalytic activity.



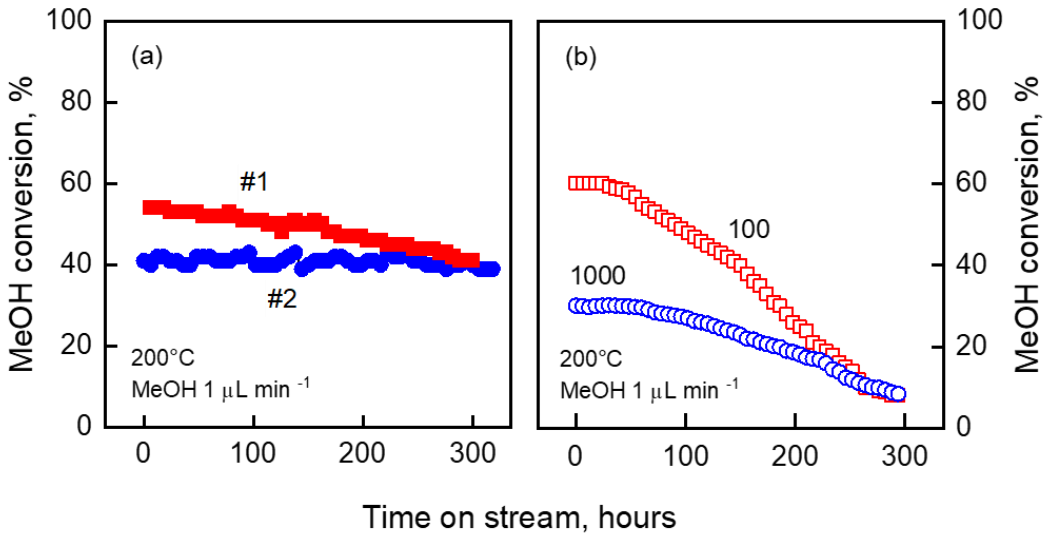


Figure 1. Performance of the membrane reactor over time for (a) bilayer and (b) single-layer membranes.

4. Conclusions

Bilayer ZSM-5 membranes markedly enhance the stability of MeOH-to-DME catalytic membrane contactors. The optimized configuration effectively limits water-induced deactivation, enabling stable operation for up to 300 h on stream. The results show that combining layers with different functional roles improves water management and catalyst lifetime during operation as membrane contactors. Overall, appropriate operation in contactor mode provides durable catalytic membrane performance for DME synthesis.

Acknowledgements

This work was supported by the European Union NextGeneration EU from the Italian Ministry of Environment and Energy Security POR H2 AdP MMES/ENEA with involvement of CNR and RSE, PNRR - Mission 2, Component 2, Investment B93C22000630006.

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THROUGH-FLOW CATALYTIC MEMBRANE CONTACTORS FOR INTENSIFIED DIMETHYL ETHER SYNTHESIS: COMPARISON BETWEEN BEA ZEOLITE AND γ-Al_2O_3 MEMBRANES – (C021)

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Keywords: dimethyl ether, catalytic membrane reactor, through-flow contactor, methanol dehydration, e-fuels.

1. Introduction

Dimethyl ether (DME) is a key e-fuel and chemical intermediate due to its clean combustion, high cetane number and potential role as hydrogen carrier. Gas-phase methanol dehydration is an attractive route for DME production, but conventional fixed-bed reactors often suffer from limited mass transfer, catalyst deactivation and incomplete selectivity. Catalytic membrane reactors operated as through-flow contactors offer process intensification by maximizing catalyst exposure and promoting product removal. This work investigates and compares two catalytic membrane contactors based on BEA zeolite and γ-Al_2O_3 membranes, aiming to assess the influence and the performance of these different catalytic systems in terms of methanol conversion, DME selectivity and long-term stability.

2. Materials and Methods

Tubular BEA zeolite and γ-Al_2O_3 membranes were integrated into catalytic membrane reactors and operated in a through-flow configuration, where the entire feed passes through the catalytic layer without selective separation. Methanol dehydration experiments were carried out over a temperature range of 200–300 °C and at different WHSVs. Reactor performance was evaluated in terms of methanol conversion, DME selectivity and productivity, including time-on-stream and regeneration tests.

3. Results and Discussion

Both membrane contactors achieved complete selectivity to DME under the investigated conditions, confirming the effectiveness of the through-flow configuration in suppressing side reactions. The BEA zeolite membrane showed high methanol conversion close to thermodynamic equilibrium at relatively low temperatures (≈200–220 °C) and higher WHSVs (Figure 1), benefiting from its strong acidity and larger micropore volume. Conversely, the γ-Al_2O_3 membrane performed optimally at higher temperatures (260–300 °C), maintaining 100 % DME selectivity with good stability and reduced deactivation by water. Time-on-stream experiments highlighted improved durability compared to conventional fixed-bed catalysts for both systems, with full recovery of activity after simple thermal regeneration. The complementary behaviour of the two membranes suggests that catalyst nature and acidity of the membranes strongly influences the process performance and stability, which, in all cases, are better than conventional reactors operated at the same conditions.



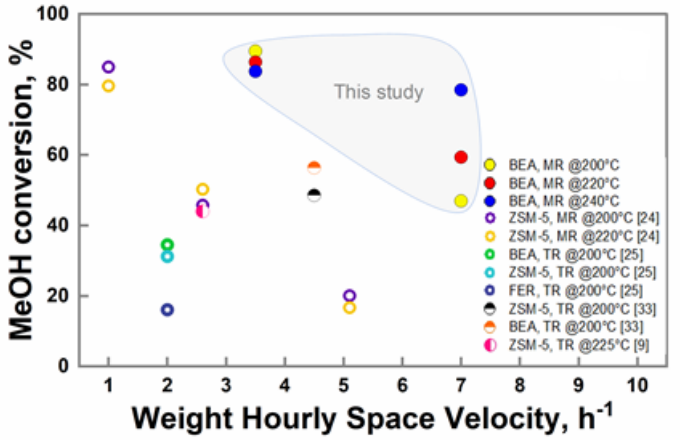


Figure 1. Performance comparison of BEA membrane reactor with conventional and membrane reactors from literature.

4. Conclusions

Through-flow catalytic membrane contactors represent an effective strategy for intensifying DME synthesis. BEA zeolite membranes enable high conversion at low temperature and high space velocity, while γ-Al_2O_3 membranes ensure excellent selectivity and stability at higher temperatures. The combined analysis highlights the flexibility of membrane-based reactors and their potential integration in sustainable e-fuel production processes.

Acknowledgements

This work was supported by the European Union NextGeneration EU from the Italian Ministry of Environment and Energy Security POR H2 AdP MMES/ENEA with involvement of CNR and RSE, PNRR - Mission 2, Component 2, Investment B93C22000630006.

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ADVANCING THERMAL ENERGY STORAGE SYSTEMS: PROGRESS OF THE ECHO PROJECT – (C022)

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Keywords: Thermal energy storage, thermochemical materials, phase change materials, residential heating and cooling.

1. Introduction

In the change toward a sustainable energy system, storage is essential to shift loads and integrate renewables. Thermal energy storage (TES) is gaining interest through advances in innovative, high-performance materials [1]. Phase change materials (PCMs) are commercially available and enable compact latent-heat systems, while thermochemical materials (TCMs) offer higher energy density and seasonal storage potential, though their instability still limits application. In this framework, the ECHO project develops a system for residential use, coupling a TCM reactor with PCM-enhanced tanks and insulation. This work presents ECHO's novelties in materials and components, as well as challenges, planned solutions and future developments.

2. Materials and Methods

ECHO follows a comprehensive approach from selection of appropriate materials to experimentation both at lab-scale and in three demonstration sites. Moreover, the work is supported and integrated by the development of an advanced control system and of an agent-based simulation at urban level. Materials were characterized by differential scanning calorimetry and scanning electron microscope, while laboratory tests and demo sites' monitoring are carried out with custom components and sensors.

3. Results and Discussion

The TCM employed in ECHO is a composite of calcium chloride and vermiculite, chosen for its stability, low cost and high porosity [2]. It is packed in drawers inside a closed reactor, fed by an air loop with a fan. A heat pump heats the charging air up to 80 °C and is followed by an electric heater to ensure complete dehydration of the TCM. During the discharging phase, in the internal loop the air is preheated and humidified, allowing the TCM to absorb water and release heat. A separate tank is used for cold storage with a eutectic PCM melting at -2.1 °C, selected for its high latent heat [3]. The ECHO TES system (Figure 1) has been built at University of Ferrara as a prototype and is optimized and demonstrated in three demo sites in Italy, Belgium and Serbia. A tailored control system with a data-driven algorithm has been developed and integrated into the system. The project is now in the phase of monitoring of the demo sites, and the first results of the one installed at CNR-ITC (Padova, Italy) are presented here, focusing on storage capacity and efficiency. Moreover, the modularity of the system is evaluated thanks to the presence of a second TCM reactor. Finally, an agent-based simulation has been carried out to evaluate the interaction of different ECHO TES systems at city level, taking into account the influence of different heat demands, electricity grids and energy markets.



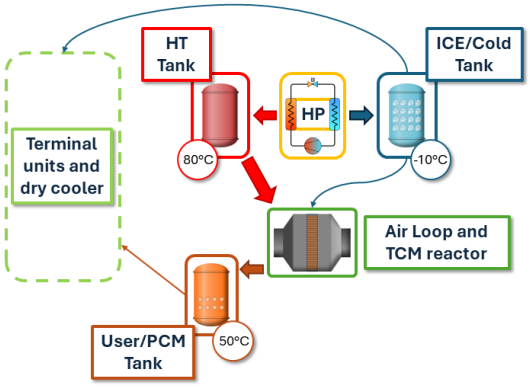


Figure 1. Simplified schematic of the ECHO TES system.

4. Conclusions

The results of the ECHO project, presented here, offer useful insights into the development of innovative and efficient TES systems, demonstrating the feasibility of the proposed solution and providing a methodological basis for future TES designs. Next steps include the completion of the monitoring campaign of demo sites and the optimization of the system's components.

Acknowledgements

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DEVELOPMENT OF HIGHLY SELECTIVE MULTICHANNEL CARBON MOLECULAR SIEVE MEMBRANES FOR HYDROGEN PURIFICATION – (C024)

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Keywords: carbon membranes, novolac resin, hydrogen separation, multichannel geometry, molecular sieving.

1. Introduction

Carbon molecular sieve membranes (CMSMs) are widely regarded as excellent candidates for high selectivity gas separation processes. This study presents a comprehensive approach to the optimization of synthesis conditions when upscaling tubular CMSMs to multichannel supports with novel geometries.

CMSMs are typically prepared through the pyrolysis of ceramic supports coated with a polymer-based solution. This solution, in tubular supports, is applied on the substrate through dip-coating procedures. The novel geometry given by multichannel supports calls for the definition of completely new fabrication conditions, specifically tailored to address the key aspects of the system.

The aim of this work is to obtain highly selective, multichannel CMS membranes, achieving the potential that has already been extensively reported in literature for tubular configurations [1]. The main feedback parameters taken into consideration are permeance and ideal gas selectivities, analyzed for H_2, N_2, CO_2 and CH_4 in a custom gas permeation setup.

2. Materials and Methods

A novolac phenolic resin was synthetized with an f/p ratio of 0.82. Coating solutions containing 25 wt% of Novolac and varying amounts of different additives were prepared, guaranteeing homogeneity with a high shear mixer. Asymmetric alumina supports with a 7-channel geometry and various pore size distributions were coated and dried, before being carbonized in a high temperature oven.

Single gas permeation tests were performed in a permeation setup at room temperature, with a feed rate of 5 nL/min and pressure difference varying between 4 and 11 bar. Membranes and synthesis materials were further characterized with various methods, including SEM, laser microscopy, elemental analysis, viscometry and TGA.

3. Results and Discussion

The established baseline performances of multichannel CMSMs, absent in literature, are defined in this study by mimicking as closely as possible the fabrication procedures of tubular CMS membranes. These results, which will define the reference membranes, point to Knudsen transport within the membrane pore structure and demonstrate an N_2 permeance in the range of 10^{-8} mol/m^2/s/Pa..

Reference membranes, in both their permeation behavior and their coating parameters, are systematically studied to determine the current bottleneck in performance. SEM imaging of the selective layers shows in some cases the presence of cracks (associated here to a high film thickness), and in general an inhomogeneous film, as presented in figure 1. The optimization of synthesis conditions and the development of novel coating solutions, using hexamethylenetetramine to effectively tune solution viscosity, has led to a leap in membrane performance. As illustrated in figure 2, optimized membranes show a strong difference in permeance between N_2 and H_2 transport, associated to a highly homogeneous selective layer. The membranes shown in figure 2 achieve an ideal H_2/N_2 selectivity of up to 20, confirming the presence of molecular sieving type transport.



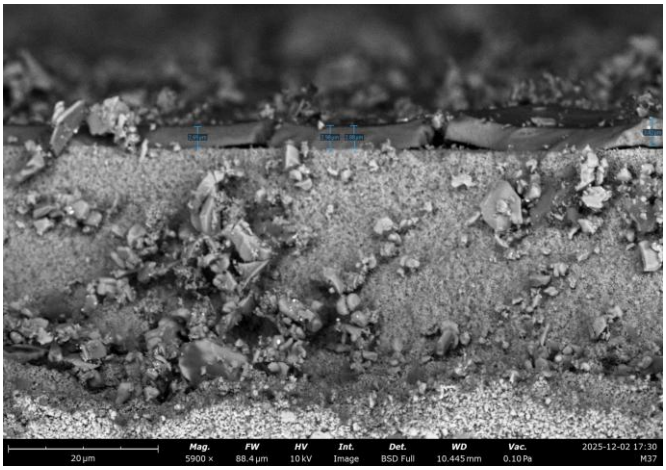


Fig. 1: SEM imaging of a cracked selective layer in a synthetized multichannel CMSM

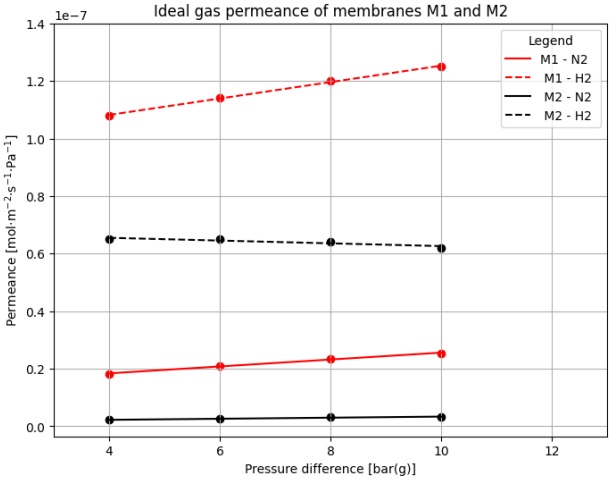


Fig. 2: H_2 and N_2 permeation curves of membranes M1 and M2.

The effects leading to this drastic improvement in performance are thoroughly investigated. TGA tests are carried out, with the objective of determining variations in carbonization behavior linked to different coating parameters. Elemental analysis is carried out, investigating the possible retention of solvent within the dry polymeric coating layer.

4. Conclusions

This work establishes a baseline performance for multichannel CMS membranes and identifies key fabrication bottlenecks. By optimizing various steps in the preparation process, homogeneous selective layers were achieved, leading to molecular sieving behavior and H_2/N_2 selectivities of up to 20. These results demonstrate the feasibility of transferring the potential of CMSMs to multichannel geometries. Future work should keep building upon these results, by further addressing scale-up challenges and validating performance under realistic operating conditions.

Acknowledgements

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CO_2 VALORIZATION INTO SYNTHETIC METHANE BY AN INTEGRATED CO_2-METHANATION REACTOR COMBINED WITH A BIO-POLYMERIC MEMBRANE SEPARATION SYSTEM: AN EXPERIMENTAL STUDY COMBINED TO EXERGY AND COST ANALYSES – (C025)

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Keywords: CO_2 valorization, methanation reaction, PLA membrane separation, exergy analysis

1. Introduction

An emerging and attracting solution for the reduction of CO_2 emissions is represented by its thermochemical conversion with H_2 into high value-added products, such as synthetic natural gas (SNG) [1]. This work proposes a novel two-stages system combining a fixed bed methanation reactor and a bio-polymeric membrane gas separation process for converting CO_2 into a synthetic CH_4 stream. At 300 °C and 3 bar, CO_2 conversion was 75%, recovering synthetic CH_4 with a concentration of 97% and CO_2 below 2%. An exergy efficiency equal to 94% was reached for the methanation reactor, 95% for the condenser and 0.01% for the membrane gas separation (MGS), determining the final cost of the synthetic CH_4 production with a value below $10/kWh operating the system between 9 and 10 h per day.

2. Materials and Methods

The schematic of the two-stages system is shown in Figure 1. In the first stage, a tubular packed bed reactor is constituted of a stainless steel type AISI 316 material, with a length of 20 cm and 1.0 cm of outer diameter. It is adopted with all the auxiliary devices to perform the methanation reaction over 3 g of 0.5% Ru/γ-Al_2O_3 catalyst. The MGS system is constituted of four cylindrical stainless steel units, housing PLA membrane samples, showing a circular shape with 4 cm of diameter.

3. Results and Discussion

In the first stage, the Sabatier reaction took place at 300 °C and GHSV = 1700 h^{-1}, converting CO_2 between 70% and 80%, depending on the adopted reaction pressure, ranging from 2 to 4 bar. The CH_4-rich stream coming out from the methanation reactor was treated in the MGS stage to recover synthetic CH_4 with a purity close to that of a typical biomethane stream. In particular, a four-stages PLA-based membrane separation system was operated at different transmembrane pressures and ambient temperature recovering CH_4 with a concentration ≥ 97%, while CO_2 and H_2 were recycled into the first stage inlet stream, ensuring a closed gas loop and preventing the release of CO_2 into the ambient. The exergy analysis revealed a maximum exergy efficiency of 94% in the methanation reactor, 95% in the condenser, and 0.01% for the MGS system, indicating that the CH_4-rich stream purification process is highly energy efficient (Figure 2). In the meanwhile, CO_2 conversion efficiency varied from ~ 60% at 2 bar to 96% at 4 bar, implying a progressively higher CO_2 capture, ranging from ~ 730 kg h^{-1} at 2 bar to ~ 1140 kg h^{-1} at 4 bar.



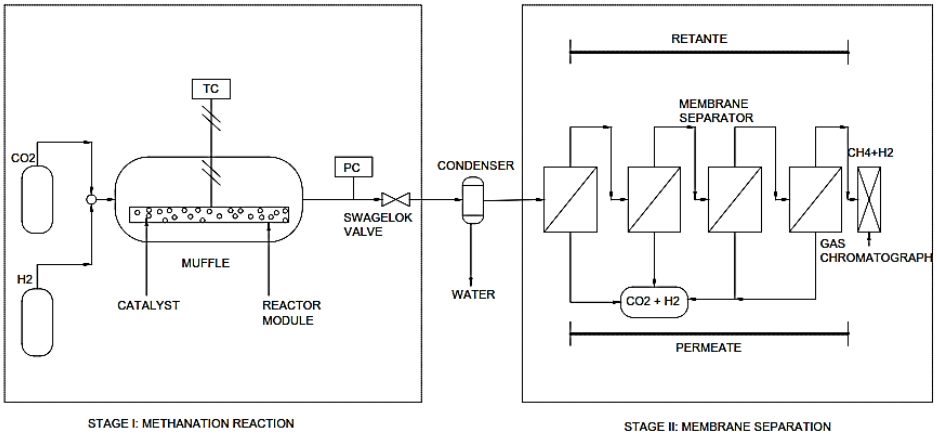


Figure 1. Two-stages system (methanation reactor + four-stages of MGS) for CO_2 conversion into synthetic CH_4

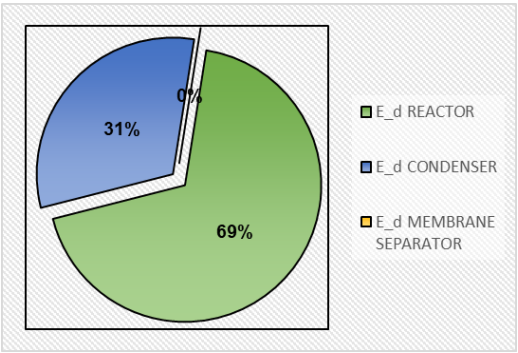


Figure 2. Exergy destruction distribution among the main components of reaction and MGS system at 300 °C and 3 bar.

4. Conclusions

This work demonstrated that if the two-stages system is operated between 9 and 10 hours a day, a synthetic CH_4 production cost below $10/kWh can be easily achieved, making the process competitive in the CH_4 market.

Acknowledgements

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IN OPERANDO HIGH-RESOLUTION LI DEPTH PROFILING IN A THIN-FILM ALL-SOLID-STATE BATTERY USING TOF-ERDA AND NEUTRON DEPTH PROFILING – (C027)

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Keywords: thin films, solid state, in operando, lithium distribution.

1. Introduction

A quantitative understanding of the Li distribution inside all-solid-state Li-ion batteries is crucial for improving electrochemical performance and interfacial stability. State-of-the-art studies rely mainly on post-mortem or surface-sensitive techniques, limiting insight into operando Li transport in buried layers. Here, we combine time-of-flight elastic recoil detection analysis (TOF-ERDA) and neutron depth profiling (NDP) to achieve high-resolution, quantitative Li depth profiling during battery operation [1, 2]. Thin-film model batteries prepared by ion beam sputtering enable controlled investigation of Li redistribution, demonstrating a novel multimodal approach for operando analysis of solid-state batteries.

2. Materials and Methods

Time-of-flight elastic recoil detection analysis (TOF-ERDA) provides quantitative, depth-resolved elemental profiles with high sensitivity to light elements such as Li, enabling nanometer-scale resolution in thin films. Neutron depth profiling (NDP) use thermal neutrons reaction with Li isotopes to non-destructively measure absolute Li concentration profiles with high accuracy. The combination of both techniques offers complementary spatial resolution and quantification for operando Li analysis.

Acknowledgements

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ENHANCING EFFICIENCY AND PROCESS OPTIMIZATION USING OPENFOAM THREE-DIMENSIONAL SIMULATION FOR INDUCTION HEATING – (C031)

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Keywords: Induction heating, OpenFOAM, 3D simulation, coils, workpiece shapes.

1. Introduction

Achieving optimal performance and energy efficiency in induction heating chemical processes requires a comprehensive understanding of the coupled fluid dynamic, thermal, and electromagnetic phenomena involved [1]. High-fidelity dynamic simulations provide a powerful tool for the design, analysis, and optimization of such processes. However, studies on induction heating that offer detailed 3D insight into magnetic field distributions and heating efficiency remain relatively scarce. In this work, we present a workflow for 3D simulation of induction heating within the OpenFOAM framework, an open-source computational fluid dynamics (CFD) modeling suite [2]. We discuss its advantages and limitations, and demonstrate its use for optimizing coil designs for inductively heated thermochemical reactors.

2. Materials and Methods

Several numerical solution steps are required to determine the heating of a workpiece located within an induction coil. The procedure consists of the following stages: (1) computation of the current density distribution in the coil; (2) solution of the magnetic vector potential throughout the domain, generated by this current density; (3). Evaluation of the eddy currents induced in the workpiece and the resulting heat generation. The solvers were implemented and compiled within the foam-extend 5.0 framework based on the work by Busse et al. (2021) [3], with additional code modifications to enable fully 3D simulations and continuous updating of temperature-dependent variables.

3. Results and Discussion

The workflow for 3D simulation of induction heating within the OpenFOAM framework is illustrated in Fig. 1a. This approach was successfully applied to prescribe the current density in complex 3D coil geometries (e.g., non-uniform or open coils), for which analytical expressions are difficult to obtain. Moreover, the ring effect of the current distribution within the coil is well captured.

Various coil and workpiece designs have been simulated and compared. The results show that the magnetic field strength along the center line of the square-tube coil is slightly higher than that of the round-tube coil (Fig. 1b). This may be attributed to the larger volume of conductor material located closer to the coil center in the square-tube geometry. In addition, the ring effect leads to a non-uniform current density when the coil tube is bent, which can further influence the resulting magnetic field inside the coil. However, its overall field strength is relatively low, and in practice, it is challenging to achieve the same uniform current distribution in a plate conductor as assumed in the simulations.

By contrast, the hairpin coil produces the weakest magnetic field. Its performance could be improved by introducing slots, analogous to those in induction motors, where slot effect enhances the field. The open coil is also of interest for induction heating studies, as the greater spacing between turns enables a thermal camera to capture the full temperature field of a catalyst bed. However, the



magnetic field within an open coil is less uniform than in a helical coil, suggesting a trade-off between a wider field of view and a more uniform magnetic field.

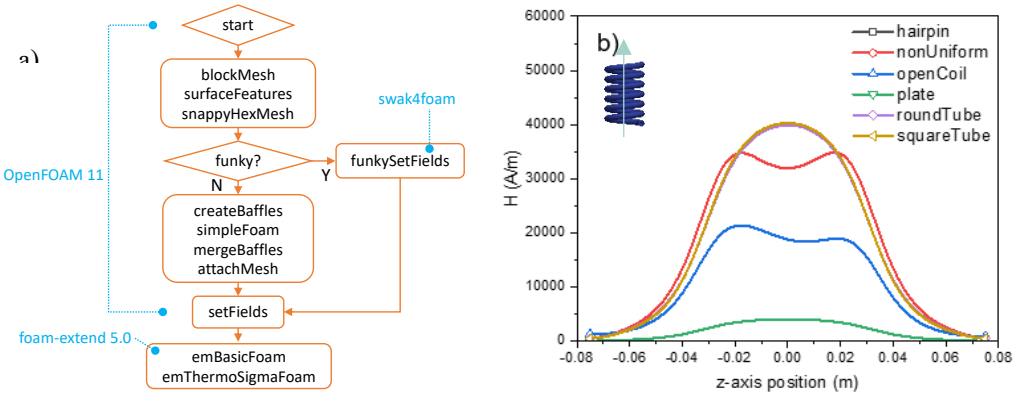


Fig. 1 a) Flow diagram of 3D OpenFOAM simulation; b) Magnetic field strength H (A/m) for different coil geometries along the center line.

4. Conclusions

Two OpenFOAM solvers were modified and applied in fully 3D simulations to model an induction-heating scenario relevant to electrical-chemical reactor heating. The solver emThermoSigmaFoam was successfully extended to incorporate temperature-dependent material properties, yielding simulated temperature distributions that qualitatively agree with experimental observations, with higher temperatures occurring at the edge of the workpiece closest to the coil. Two distinct approaches were developed to prescribe the current density within the internal field of the 3D coil. Among these, the simpleFoam-setFields approach appears particularly promising for representing the current distributions in complex 3D geometries. To maximize the induced power for induction heating of chemical reactors, careful selection of the workpiece geometry, current density, and operating frequency is essential. Overall, the results demonstrate clear potential to optimize both coil and workpiece geometries to achieve efficient, spatially uniform heating in chemical reactors.

Acknowledgements

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IMPROVED ELECTROLYTIC CELL PERFORMANCE USING LASER-TEXTURED Ni-FELT – (C032)

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Keywords: Laser surface micro-/nanostructuring, Anion-Exchange Membrane Water Electrolysis, Laser Induced Periodic Surface Structures,

1. Introduction

Micro- and nanostructured surfaces with tailored wettability are widely employed in numerous applications. In this context, Laser-Induced Periodic Surface Structures (LIPSS) represents a powerful approach for finely tuning surface morphology and wettability. When processing fragile materials, ultrashort laser pulses are advantageous, for their capability to reduce the risk of thermal damage, while ensuring high accuracy and reproducibility. Here, we textured Ni-felt sheets used as an element of the anion-exchange membrane (AEM) of electrolytic cells, for hydrogen production [1]. The primary objective was to enhance the intrinsic hydrophobicity of pristine Ni-felt in order to improve the interfacial interaction with the membrane, while preserving the integrity of the individual fibers.

2. Materials and Methods

A fs laser was used to generate LIPSS on Ni-felt. Their wettability was interpreted through a hierarchical Cassie-Baxter model, where LIPSS define an effective microscale contact angle governing the final wetting behavior.

MEAs based on a Piperion membrane were prepared by cold pressing, i.e., anode: bare or laser-processed Ni felt; cathode: Pt-based GDE (0.2 mg cm^{-2}). Electrochemical tests in terms of LSV, EIS, and a 70 h stability test were performed in a 5 cm^2 AEM-WE cell.

3. Results and Discussion

After the laser texturing process, wettability was measured to highlight the influence of laser parameters on the contact properties of the processed samples. A marked improvement in hydrophobicity (WCA = 153°) was obtained through the laser treatment (WCA≈125° for bare Ni-felt). Their wettability was also analyzed using a hierarchical multiscale approach combining experimental measurements, SEM analysis, and wetting models. The double-scale morphology of LIPSS over Ni-felt was approximated by an array of cylindrical crests over the fibers. Thus, LIPSS define an effective microscale contact angle obtainable from the analytical solution for cylindrically textured surfaces used into the Cassie-Baxter model [3], leading to a macroscopic angle of ~150°, in excellent agreement with the experimental value.

Superhydrophobic Ni-felt sheets were implemented in AEM-WE (in Figure 1, their electrochemical performances). The laser-processed MEA achieved a much higher current density at an operating voltage of 2.2 V compared to the untreated reference (see Figure 1 a). This enhanced performance is likely associated with improved electrode kinetics and interfacial properties. Indeed, EIS measurements (inset of Figure 1a) revealed a noticeable decrease in the charge-transfer resistance for the laser-treated electrode, which suggests more efficient electrochemical reactions and improved electron and ion transport at the electrode-electrolyte



interface, ultimately contributing to the observed increase in current density. Moreover, a short-term stability test was conducted, revealing that the electrochemical performance remains stable throughout the entire duration of the test, with no significant degradation in cell voltage (Figure 1b). This stable behavior confirms that the laser treatment enhances the initial performance of the MEA and contributes to maintaining its electrochemical efficiency under continuous operation.

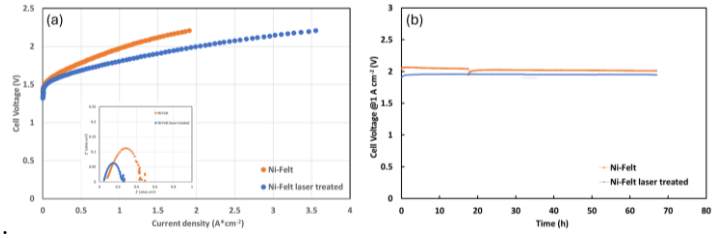


Figure 1. I-V curves (a) and short stability test (b) comparison of the tested MEAs at 80°C.

4. Conclusions

Ultrashort-pulse laser texturing enabled the controlled formation of LIPSS on Ni-felt without damaging the fibers, significantly enhancing surface hydrophobicity. Optimized processing conditions yielded superhydrophobic behavior and improved electrode performance in AEM water electrolysis, improving the interfacial interaction with the membrane and reducing the charge-transfer resistance, and increasing the maximum current density.

Acknowledgements

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3D MULTIPHYSICS MODELING OF REVERSIBLE SOLID OXIDE BOTTOM CELL – (C036)

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Keywords: rSOFC, Multiphysics modelling, Degradation mechanisms, Electrochemical analysis,

1. Introduction

3D multiphysics modelling is essential for understanding degradation phenomena in solid oxide fuel cells (SOFCs), as it allows the coupling of current distribution, electrochemical reactions and thermal gradients, which are direct causes of thermomechanical and electrochemical stress. Current scientific literature highlights a significant lack of correlation between the experimental performance of rSOFCs and the related computational models [1]. The originality of this work lies in the integration of these aspects for the study of innovative materials that have never been used before. The objective is to characterise and design an rSOFC model that allows the analysis of critical degradation parameters in order to identify operational strategies that minimise their impact on long-term performance.

2. Materials and Methods

The proposed model reproduces an electrolyte-supported button cell (Ø 25 mm) with standard materials (Ni-YSZ, YSZ, LSCF-SDC) and SDC interlayer. The methodology combines charge, mass and energy transport using Fuel Cell and Heat Transfer modules [2]. Electrochemical kinetics are described by Butler-Volmer equations, while transport in porous matrices follows Maxwell-Stefan and Fick models. The computational framework assumes steady state and ideal gas behaviour for material validation.

3. Results and Discussion

The results show that the model was successfully validated through direct comparison between the simulated polarisation curves and experimental data extracted from the literature for standard configurations. The simulated curve shows quantitative and qualitative alignment with the experimental data, confirming the accuracy of the computational framework in predicting the electrochemical response of the cell.

Subsequently, the study focused on modelling degradation in relation to variations in gas composition, temperature and overpotential across the electrodes. These parameters represent the main triggers of deterioration mechanisms, and the model results show excellent agreement with experimental data.

4. Conclusions

This work demonstrates that a 3D multiphysics model can reliably capture the electrochemical behaviour and degradation factors of rSOFC cells.



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EXPERIMENTAL ASSESSMENT AND SYSTEM-LEVEL ANALYSIS OF ALUMINUM-BASED HYDROGEN STORAGE – (C037)

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Keywords: Aluminum-steam reaction, Hydrogen, Experimental, Energy storage, System modeling.

1. Introduction

The increasing penetration of renewable energy sources calls for safe, energy-dense, and scalable solutions for long-term energy storage. Among metal-based energy carriers, aluminum is particularly attractive due to its high volumetric energy density, abundance, and ease of storage and transport [1]. When oxidized with steam, aluminum produces hydrogen and releases significant thermal energy, enabling combined hydrogen production and power generation [2]. Experimental data on high-temperature aluminum–steam reactions and their system-level implications are limited. This work investigates aluminum-based hydrogen storage through an integrated experimental and modeling approach, aiming to assess its potential for Power-to-Power applications and district-scale energy systems.

2. Materials and Methods

High-temperature aluminum–steam oxidation was experimentally investigated in a tubular microreactor operating up to 1000 °C under both isothermal and temperature-programmed oxidation (TPO) conditions. Hydrogen production was continuously monitored, and aluminum conversion was quantified. Experimental results were implemented into a system-level model of an aluminum-fueled cogeneration plant integrating a solid oxide fuel cell, gas turbine, and steam cycle. A district-level case study was developed to evaluate round-trip efficiency, transport impacts, and CO_2 emissions.

3. Results and Discussion

Experiments showed aluminum conversions up to 76% during TPO tests and 50–65% under isothermal conditions between 900–1000 °C. Particle size strongly affected reaction rates, while global hydrogen yields were comparable at high temperature. System simulations highlighted a strong linear dependence of plant efficiency on aluminum conversion, with electrical efficiencies up to 57% (LHV-based) using experimental data and up to 87% for ideal conversion. The Rankine cycle contribution decreased significantly at high water excess, becoming ineffective beyond ~350%. District-level analysis revealed lower round-trip efficiency compared to compressed hydrogen storage (24–35%), but a fourfold reduction in transport energy consumption due to aluminum's high energy density.

Table 1. Exemplary results from TPO experiments.

Powder type	H_2 yield (ml/g)	Al conversion (%)	H_2 yield (ml/g) at T < 660 °C	Al conversion (%) at T < 660 °C
Coarse	945	76	69	6
Fine	920	74	221	18



4. Conclusions

This work provides a comprehensive assessment of aluminum as a solid hydrogen carrier, combining high-temperature experiments with system-scale simulations and district-scale analyses. Results demonstrate the technical feasibility of aluminum-based Power-to-Power systems and highlight key trade-offs between efficiency, water management, and transport benefits. Future work will focus on reactor scale-up and demonstration of the Al–H_2O process, optimization of reaction parameters in the medium-high temperature range, and integration with carbon-free aluminum production routes to enhance efficiency and sustainability. While current aluminum production routes limit overall carbon neutrality, emerging carbon-free smelting technologies could make aluminum a competitive and scalable energy storage solution for future renewable energy systems.

Acknowledgements

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ZEOLITE-TEMPLATED CARBONS AS EFFECTIVE SUPPORTS FOR BOOSTING COPPER CATALYST FUNCTIONALITY IN CO_2-TO-METHANOL PRODUCTION – (C038)

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Keywords: ZTC; methanol; green hydrogen; CO_2 conversion; Cu catalysts.

1. Introduction

Among the available technological routes to turn captured CO_2 into sustainable fuels, catalytic CO_2 hydrogenation to methanol stands out as a particularly attractive option [1]. In this context, CuZnZr catalysts have emerged as promising alternatives to conventional CuZnAl systems, owing to the beneficial role of ZrO_2 in the heat management along the catalytic bed, also ensuring an extended catalyst lifetime in presence of the water formed during operation [1]. Nevertheless, to enhance CO_2 activation at low reaction temperature, the use of functional supports, like the zeolite-templated carbon frameworks (ZTCs), has been recently proposed as effective to increase the local concentration of reactants in the vicinity of active sites, taking advantage from their peculiar texture properties and exceptional CO_2 adsorption capacity [2]. In this work, we investigate a composite catalyst that integrates a previously optimized CuZnZr formulation with the unique features of ZTCs, aiming to enhance CO_2 availability while preserving the intrinsic functionality of the metal-oxide phase during methanol synthesis.

2. Materials and Methods

The CuZnZr catalyst (CZZ) was synthesized by gel-oxalate coprecipitation of the nitrate precursors, with a nominal Cu/Zn/Zr atomic ratio of 60/30/10. On the other hand, ZTC was prepared by chemical vapour deposition of a carbon matrix into the porous structure of a beta-zeolite (Si/Al, 25), as described elsewhere [3]. The CZZ/ZTC composite catalyst was finally prepared by mechanical mixing of the two parent CZZ and ZTC materials.

Catalytic performance of the composite CZZ/ZTC catalyst was evaluated in a continuous-flow fixed-bed reactor, by comparing the observed activity-selectivity pattern against the parent CZZ catalyst taken as a reference. Prior to reaction, the catalysts were reduced under pure hydrogen at 300 °C for 1 h. CO_2 hydrogenation tests were carried outat a total pressure of 30 bar over a temperature range of 200–260 °C, by employing an H_2/CO_2 molar ratio of 3:1 and a gas hourly space velocity of 8,800 *N*mL g_{cat}^{-1} h^{-1}.

3. Results and Discussion

X-ray diffraction (XRD) shown in Fig. 1 (Left) clearly reveals the diffraction peaks corresponding to tenorite (CuO) and zincite (ZnO) in all the investigated CZZ-based samples. At the same time, the characteristic features of the zeolite-templated carbon framework remain visible in the composite material, indicating that both the crystalline oxide phases and the ZTC structure are preserved upon composite formation.

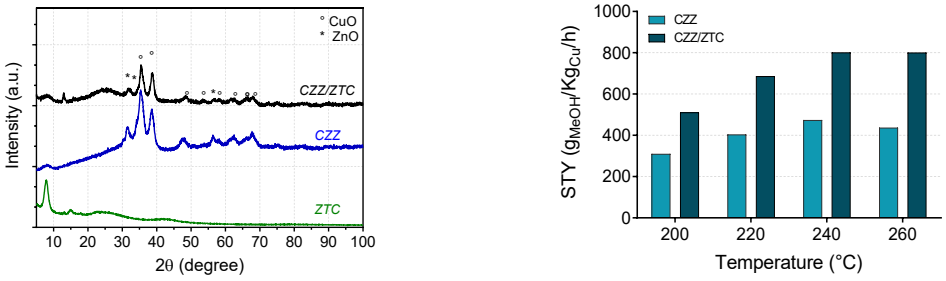


Figure 1. (Left) XRD patterns of the investigated samples. (Right) STY as a function of reaction temperature.



To determine the effect of the ZTC framework on the performance of the CZZ catalyst, the methanol space–time yield (STY) of the composite CZZ/ZTC system and the reference catalyst was normalized to the copper content and plotted as a function of reaction temperature, as shown in Fig. 1 (Right). As observed over the temperature range investigated (200-260 °C), the CZZ/ZTC catalyst consistently exhibits a higher methanol STY compared to the reference CZZ system, with the productivity becoming more pronounced at elevated temperatures. This improved performance can be basically ascribed to a better dispersion of the active phase, favoured by the increased accessible surface area provided by the ZTC framework, which finally enables a more effective activity-selectivity pattern and enhanced catalytic efficiency under the explored reaction conditions.

4. Conclusions

This study demonstrates that zeolite-templated carbons can be successfully integrated with Cu-based catalysts to enhance methanol synthesis via CO_2 hydrogenation. The composite CZZ/ZTC systems exhibit improved process productivity while preserving the structural integrity and redox properties of the mixed oxide phase. As frameworks with specific CO_2 affinity, rationally designed ZTC materials can really promote a more efficient utilization of surface sites, thereby unlocking the potential of composite catalytic architectures for sustainable carbon conversion and production of e-fuels.

Acknowledgements

This work was funded through the programme agreement between the Italian Ministry of Environment and Energy Security (MASE) and ENEA on the topic “Ricerca e sviluppo sull’idrogeno” (AdP POR H2, PNRR M2C2, Inv. 3.5), with the involvement of CNR and RSE. Additional support was received from the Italian Electrical System Research programme (MASE, Integrated Project “Technologies and End-Uses of Hydrogen”, Implementation Plan 2025–2027) and from the GREENCAT project (P2022KA5ZZ_PE8, PRIN PNRR 2022, M4C2, Inv. 1.1).

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A DUAL SUSTAINABILITY PERSPECTIVE ON PHOTOELECTROLYSIS: INTEGRATED ENVIRONMENTAL AND ECONOMIC LIFE CYCLE ASSESSMENT OF GREEN HYDROGEN PRODUCTION – (C044)

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Keywords: Green Hydrogen, LCA, eLCC, Photoelectrolysis,

1. Introduction

This work consists of a Life Cycle Assessment (LCA), performed according to ISO 14040/44 standards and an environmental LCC (eLCC) [1-2] analysis of a novel photoelectrolysis cell, using a cradle-to-gate approach to help designers make environmentally sustainable and economically viable choices. The calculations were performed on a laboratory prototype cell having an area of 10 cm², and then scaled up to a commercial cell of 80 cm².

2. Materials and Methods

The LCA was conducted using SimaPro 9.6 with Ecoinvent 3 data and the ReCiPe 2016 Midpoint (H) method. The functional unit comprised a single assembled cell, incorporating an anode on FTO glass, a cathode, a polymer membrane and a PVDF casing.

The LCC analysis encompassed the calculation of capital expenditures (CAPEX) and operating expenditures (OPEX). In particular, the Net Present Value (NPV) was calculated in order to assess the economic viability of the investment.

The eLCC was based on the "Environmental Price" (EP) [3] approach, which expresses the willingness to pay for less pollution in euros per kilogram of pollutant considering the Climate change category.

3. Results and Discussion

The results indicate that climate change, human toxicity and terrestrial ecotoxicity are the most relevant impact categories. In normalized terms, human carcinogenic toxicity clearly dominates the environmental profile, reaching a value of $3.34 \cdot 10^{-2}$, followed by freshwater ecotoxicity ($1.31 \cdot 10^{-2}$) and marine ecotoxicity ($9.81 \cdot 10^{-3}$). Terrestrial ecotoxicity also shows a non-negligible contribution ($1.46 \cdot 10^{-3}$), whereas climate change impacts, although relevant ($3.86 \cdot 10^{-4}$), are lower compared to toxicity-related categories (Fig. 1). The primary areas of concern relate to the anode process and fluoropolymer materials, due to high energy consumption and the production of fluorinated compounds. Membrane, casing and assembly stages contribute less significantly.



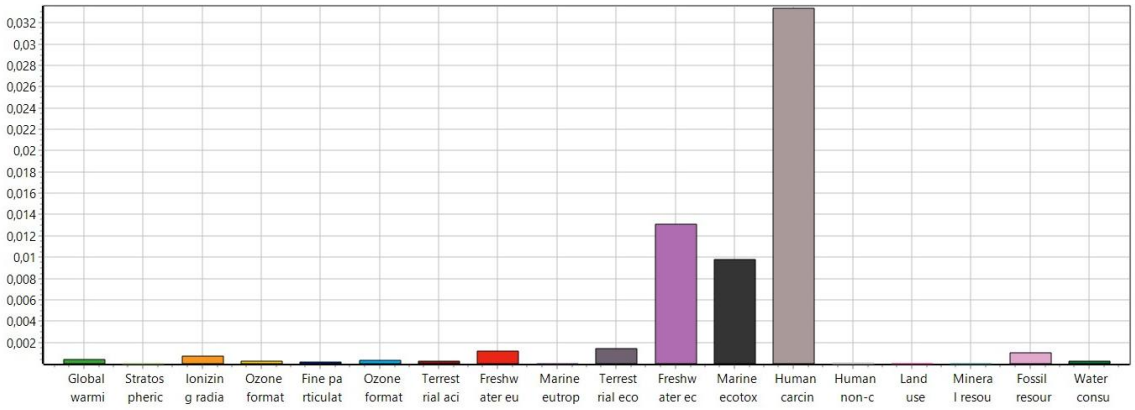


Fig. 1: LCA results using the ReCiPe 2016 midpoint normalised method.

Despite the low technology readiness level (TRL), the study simulated a realistic production and commercialization process. The analysis assumed a semi-artisanal production, with production volumes not exceeding 4,000 units per year. The target market includes not only industry, but also research institutions commissioning cells for experimental applications. In this context, the identification of environmental hotspots provides a consistent basis for the economic assessment, enabling a direct link between environmental burdens and cost drivers within the integrated LCC and NPV analyses. The NPV calculation showed that the break-even point was reached within 3.5 years. Considering externalities as additional costs affecting the production value of the photoelectrolysis cell, the incidence of each cost category is: Capex 91.98%; Opex 7.94%; Climate change (EP) 0.08%.

4. Conclusions

The study emphasises the pressing requirement to minimise the energy intensity of anode production and to replace fluoropolymers with more environmentally friendly alternatives. These measures are essential for steering the development of photoelectrolytic cells towards more sustainable and scalable technologies. To optimise the environmental performance of the device, energy consumption during heat treatments should be limited and the use of low-impact materials integrated.

The product and production process under investigation can be defined as virtuous and sustainable in terms of environmental impact, representing an investment with a good potential return in purely economic terms.

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CATALYTIC DEHYDROGENATION-HYDROGENATION OF ORGANIC CARRIERS FOR CLEAN HYDROGEN GENERATION AND STORAGE: EXPLOITATION OF DIFFERENT BIO-MOLECULES AND CATALYST OPTIMIZATION – (C047)

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Keywords: clean hydrogen, catalytic dehydrogenation-hydrogenation, LOHC, bio-molecules.

1. Introduction

Hydrogen is at the core of Scientific Communities' debates since it is considered the most versatile energy carrier able to ensure a substantial and definite conversion towards a net-zero energy system. Although the impressive number of novel researches on the field of hydrogen technologies, some issues regarding the costs of hydrogen production, storage and transportation still remains, making not fully available its exploitation at large scale. As cost-effective and promising alternative to water electrolysis, the catalytic dehydrogenation-hydrogenation of organic molecules "hydrogen-rich" has gained considerable attention, for both the production and storage of hydrogen. In this work, different organic molecules will be employed in the dehydrogenation-hydrogenation processes evaluating the effect of the chemical structure of the feedstock and the influence of the operative condition on the process performance and hydrogen yield. Moreover, the choice of the catalytically active elements will be oriented towards the use of non-toxic and CRMs-free species, aiming at pushing the hydrogen generation even more sustainable and economically viable.

2. Materials and Methods

Supported multi-metallic catalysts were prepared through co-precipitation and incipient wetness impregnation synthesis route. Prior to catalytic testing, catalysts were *in-situ* reduced under 60ml/min of pure H_2 or H_2/H_2S mixture at 400°C for 4h. The dehydrogenation tests were carried out by using a laboratory semi-automatized micro-plant at 250-400°C and 1-5 bar, feeding 40 $cc.min^{-1}$ of inert N_2 carrier and 0.003 ml/min of liquid hydrocarbons. The hydrogenation tests were carried out at 12-180°C and 20 bar, feeding 5 $cc.min^{-1}$ of H_2 and 0.01 ml/min of liquid hydrocarbons. In each test, the reactor was loaded with 2g of catalyst (10-16 mesh) diluted one-to-one with quartz pellets. The on-line composition of reactants and products was determined by using a GC Agilent model 8890A equipped with a thermo-conductivity (TC) and a flame ionization (FI) detector.

3. Results and Discussion

The catalytic performance of a high-load Fe catalyst (Fe95) in the dehydrogenation of cyclohexene, for the hydrogen generation process, demonstrates a strong dependency on operating temperature. As shown in Figure 1a, Fe95 shows a progressive increase in H_2 generation rates and cyclohexane conversion as temperature rises from 250 to 400°C, with the extraction efficiency reaching a maximum of 15%. The combination of Cu with Fe is expected to improve the dehydrogenation capacity of the systems.



Then, in the hydrogenation phase, evaluated through the hydrogenation of 1,4-cyclohexadiene over NiMo-based catalyst, the reference catalytic system shows a good activity at low temperatures, reaching a complete diene conversion at 180°C. However, NiMo-ref. catalyst favors the formation of the cyclohexene product, not allowing the complete hydrogenation of the molecule. This leads to a maximum storage yield of 26 g_{H2}/kg_{LOHC}, which corresponds to the 53% of the total storage capacity of the system (Figure 1b).

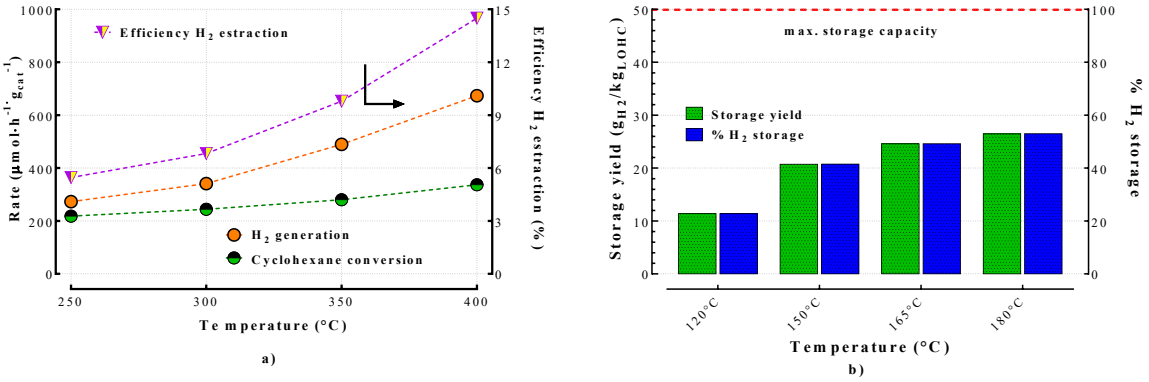


Figure 2. a) catalytic data in the dehydrogenation of cyclohexene over Fe95 catalyst; b) catalytic data in the hydrogenation of 1,4-cyclohexadiene over NiMo-ref. catalyst.

4. Conclusions

The practical exploitation of bio-molecules both for the clean hydrogen production and chemical storage has been assessed. FeCu-based catalyst showed a good activity in the dehydrogenation of organic molecules while NiMo-based one were selected for the hydrogenation process. Noble metal-based catalysts were reported for comparison.

Acknowledgements

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SCALABLE PRODUCTION OF Pt CATALYST EMBEDDED IN NANOSCALE CARBON NETWORK FOR DURABLE FUEL CELLS – (C048)

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Keywords: PEMFC, catalyst, durability, one-step synthesis.

1. Introduction

Proton exchange membrane fuel cells (PEMFC) suffer significant voltage degradation at lower Pt loadings on the cathode. Expedited commercialization and sustainable utilization of scarce resources demand highly durable Pt-based electrocatalysts produced via rapid, scalable processes. This presentation focuses on mitigating durability limitations of PEMFC MEAs by proposing sustainable solutions how to overcome them at low Pt loadings <0.15 mg cm^{-2} (CCL). Specifically, our study focuses on highly durable catalyst prepared using flame spray pyrolysis (FSP) which is a versatile resource-lean gas-phase synthesis technique for rapid and scalable production of materials in one-step (see Figure 1 (left panel)) [1]. The applicability of this technique to synthetize catalyst of electrochemical devices was already successfully demonstrated in PEM electrolysis [2]. In this study, the technique was extended to be used for the synthesis of carbon encapsulated Pt catalyst for ORR in PEMFC. We present a functional electrocatalyst consisting of Pt NPs embedded in nanoscale carbon network (denoted as Pt-e-Cn) prepared by FSP (Figure 1). Using the ORR as a model reaction, we demonstrate its high activity and excellent durability after proper catalyst activation in a practical PEMFC with a low Pt loading of 0.15 mg cm^{-2} at the cathode. Through a combination of electrochemical and microscopy tools, the strong impact of the nanocomposite on the catalytic durability is highlighted.

2. Materials and Methods

Pt-e-Cn with a (29±1) wt.% Pt was synthesized using FSP techniques. precursor solution containing Platinum (II) acetylacetonate dissolved in xylenes (the primary carbon source) at a final Pt concentration of 25 mM was atomized at a flow rate of 4 mL min^{-1}. The spray was ignited by a support flame fueled by 1 L min^{-1} CH_4 and 2 L min^{-1} O_2, generating a high temperature spray flame. With a 12 min FSP run, approximately 0.5 g of Pt-e-Cn was collected on a sampling glass fiber filter (GFF) disk positioned 60 cm above the atomizer and used without further processing. The catalyst inks were prepared by dispersing catalyst powder in a solvent mixture of water and isopropanol with an ionomer solution (Nafion D521) using an ultrasonic homogenizer. Nafion NRE 211CS membrane with a thickness of 25 µm was used as the PEM. MEAs with 4 x 3 cm^2 active area were prepared by sandwiching the CCMs between commercial gas diffusion layers (GDL) with a micro-porous layer (MPL). A 12 cm^2 differential cell from Baltic fuel cells was used for the experiments. All tests were conducted at 80 °C and 80% RH.

3. Results and Discussion

Results at MEA level (see Figure 1 (right panel)) demonstrate high stability in accelerated stress test (AST) conditions due to the unique structure of the catalyst with Pt particles embedded in a thin carbon layer. The results are benchmarked versus AST carried



out using MEAs prepared identically, but with commercial Pt/C catalyst. While performance penalties are almost negligible, the MEA with FSP catalyst exhibits clearly higher stability. Hence, this approach can increase MEA lifetime, an aspect of particular interest for heavy-duty application and, in addition, has high potential in terms of technology transfer to the industry due to straightforward scalability. Pt-e-Cn demonstrates exceptional durability with only a negligible 3% loss of BOT performance at 0.5 V and a slight gain at 0.8 V, suggesting potential access to additional Pt surface. Also ECSA surface loss was measured to be significantly lower than a reference commercial Pt catalyst with identical testing conditions.

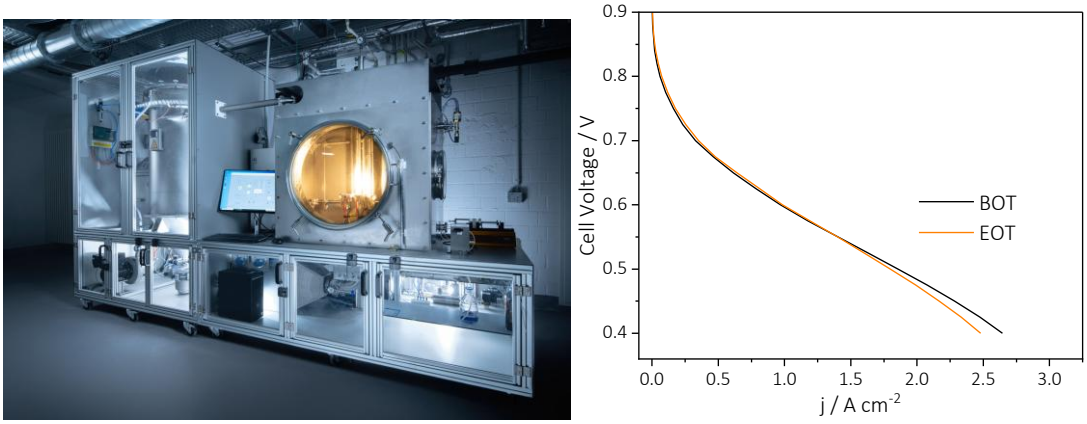


Figure 1: (Left) FSP facility at DLR. (Right) H2-air fuel cell polarization plots at BOT (activated) and at EOT (after 30k cycles AST for catalyst).

4. Conclusions

We present a functional high-surface-area carbon nanonetwork-embedded catalyst structure produced via a highly scalable and cost-efficient FSP technique in a single process step. Upon proper activation, the gas-phase-produced, highly dispersed Pt nanocatalysts (≈2 nm) show exceptional durability, and uncompromised performance after >1k AST. It retained 97% of power output at 0.5 V and 88% of ECSA after extensive durability testing in a low-Pt-content PEMFC – significantly outperforming the start-of-the-art catalyst, which retains only 65% and 35%, respectively.

Acknowledgements

The research leading to these results was supported by the project SUSTAINCELL (101101479) which is supported by the Clean Hydrogen Partnership and its members Hydrogen Europe and Hydrogen Europe Research.

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SUSTAINABLE AQUEOUS SYNTHESIS OF MIL-100(Fe): A PROMISING MOF FOR WATER SORPTION APPLICATIONS – (C049)

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Keywords: Metal-Organic Frameworks, green synthesis, porous materials.

1. Introduction

Metal-Organic Frameworks (MOFs) are crystalline porous materials composed of metal ions coordinated with organic linkers, with exceptionally high surface areas (up to 7000 m^2/g) and tunable pore architectures. These features make MOFs highly promising materials for sorption applications. Traditional MOF synthesis relies on energy-intensive solvothermal methods (150-220°C) using non–environmentally friendly solvents (*e.g.,* HF, DMF) hindering scalability. This work investigates a greener route by room-temperature aqueous MIL-100(Fe) synthesis. The MOF shows measurable water uptake at low humidity (0.02–0.05 g/g at 5% RH) [1] and is particularly promising due to the availability of cost-effective, for sustainable water harvesting in arid regions.

2. Materials and Methods

MIL-100(Fe) was synthesized by an aqueous green route: $FeSO_4$ $7H_2O$, trimesic acid, and NaOH were dissolved in deionized water, stirred overnight, then filtered and dried at 120 °C. Structural characterization was performed by X-ray diffractometry (XRD) to confirm crystallinity and phase purity. Surface area and pore volume were determined by means of N_2 physisorption. Sorption capacity performance was measured using a Dynamic Vapor Sorption (DVS) analyzer at 30 °C in a relative humidity range of 0–70%.

3. Results and Discussion

Several batches were produced to test the reproducibility of the manufacturing process. XRD analysis confirms the successful formation of the MIL-100(Fe) crystalline framework, showing the characteristic reflections associated with the Fe_3-O cluster–based porous structure. The sharp and well-defined peaks indicate high crystallinity and the absence of detectable secondary phases.

BET measurements reveal a specific surface area of approximately 1362.49 m^2/g and pore volume of 0.66 cm^3/g consistent with values typically reported for well-structured MIL-100(Fe). The N_2 adsorption isotherm exhibits a type-I profile, confirming the presence of a developed microporous network.

DVS analysis highlights a strong affinity with water vapor, with a maximum uptake of ~ 0.55 g/g at high relative humidity. The hysteresis observed between adsorption and desorption cycles highlight the probable presence of coordinatively unsaturated metal sites and partial water retention within narrower pores [2].

The data obtained for the material produced by the proposed green route were compared with the one reported in



literature for the same material obtained with a common industrial route (surface area of 1519 m^2/g, pore volume of 0.81 cm^3/g, and a maximum water uptake of 0.60 g/g.) [3]. This comparison was pivotal to confirm the effectiveness of the synthesis process in terms of water uptake, porous structure and crystallinity. Overall, the synthesized MIL-100(Fe), produced by the green route, is shown to have similar properties to the industrial one. Indeed, it possesses ordered structure, high surface area, and good interaction with polar molecules, while at the same time reducing the environmental impact, making it a promising candidate for adsorption processes such as for applications thermochemical energy storage, water harvesting, sorption desalination.

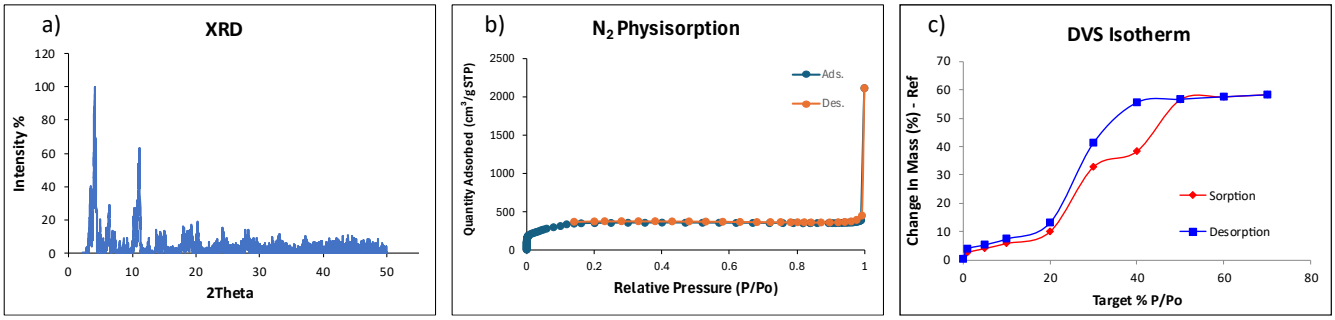


Figure 1: Results of the performed analyses: a) XRD, b) N_2 physisorption and c) DVS Isotherm.

4. Conclusions

The green synthesis of MIL-100(Fe) produced a material with an ordered structure, good porosity, and an adsorption capacity comparable to the industrial route. The results confirm the effectiveness of the method and suggest its use in applications such as water harvesting and energy storage, with future studies aimed at process optimization.

Acknowledgements

This work has been funded by European Union—Next Generation EU, Mission 4 Component 2, Investment 1.1—Call Prin 2022 PNRR—Directorial Decree n. 1409 of 14-09-2022, Project: INSTINCT—INnovative Sorbent maTerIals and techNologies for low-Carbon heating and waTer provision. CUP: J53D23015690001—ID code: PRIN_2022PNRR_P2022CRXAM_001.

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PGM-FREE METAL-FUNCTIONALIZED TiO_2 NANOTUBES ELECTRODES FOR ALCOHOL OXIDATION TOWARD COUPLED GREEN HYDROGEN AND VALUE-ADDED CHEMICALS PRODUCTION – (C052)

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Keywords: Alkaline electrolysis, Alcohol oxidation, Green hydrogen and value-added products, PGM-free electrocatalysts, TiO_2 nanotube electrodes

1. Introduction

The efficiency of alkaline water electrolysis is limited by the sluggish oxygen evolution reaction (OER). Replacing OER with alcohol electrooxidation offers a valuable route to reduce energy demand while enabling the co-production of value-added chemicals. Recent studies have shown that PGM-free catalysts can efficiently drive glycerol oxidation [1] or methanol oxidation [2] to enhance green hydrogen production efficiency. However, the development of stable, high-surface-area and scalable PGM-free electrodes remains challenging. In this work, we report PGM-free metal-functionalized TiO_2 nanotube electrodes fabricated via electrodeposition, designed to promote alcohol oxidation toward green hydrogen and value-added products in alkaline electrolysis.

2. Materials and Methods

TiO_2 nanotubes (NTs) were prepared using a Ti fiber felt as substrate and a two-step method which includes an anodizing step and then a thermal treatment (annealing step). Electrocatalytic layers were prepared by a potentiostatic electrodeposition, using NTs as substrate, and Ni and/or Co-based salt-containing aqueous electrolyte. Electrodes were characterized by SEM and EDX, and by LSV and EIS in alcohol-containing alkaline environment. Stability tests were carried out to test electrodes durability and estimate Faradaic efficiency toward hydrogen and value-added products generation.

3. Results and Discussion

Substrate for electrodeposited electrocatalytic layer was prepared by anodizing Ti felt to form TiO_2 NTs. To make NTs prone to host metallic particles, NTs with an average diameter of 120 nm and an average length of 700 nm were obtained, with walls ~ 15 nm thick. Substrate geometry should allow high surface area for electrocatalytic layer, leading to better electrochemical performance, and, at the same time, high chemical stability in alkaline conditions, since TiO_2 is highly stable in alkaline environment.

Electrode potential for electrodeposition was chosen after recording cyclic voltammetries carried out in Ni and Co-containing electrolytes using TiO_2 NTs electrode. Electrodeposition conditions were then optimized testing several operating conditions, i.e. applied potential and time, to have maximum electrochemical performance toward methanol oxidation reaction (MOR) and glycerol oxidation reaction (GOR). The comparison of LSVs recorded using functionalized TiO_2 NTs electrode in methanol-containing, glycerol-containing and alcohol-free alkaline electrolytes is reported in Figure 1.



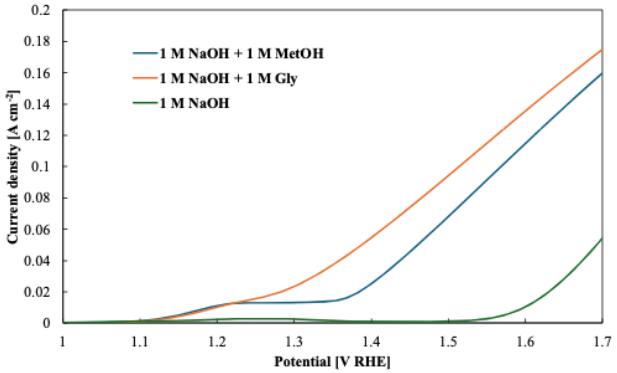


Figure 1. LSV recorded by using NiCo-based electrode in 1 M NaOH aqueous solution with and without alcohol.

In alcohol-free alkaline electrolyte, i.e. 1 M NaOH aqueous solution, an oxidation peak can be observed at ~ 1.25 V vs RHE, related to the formation of hydroxide or oxyhydroxides species, and then the onset of OER can be observed at potential more anodic than 1.5 V vs RHE. It is worth noting that, in presence of glycerol-containing electrolyte, a current density of 100 mA cm^{-2} can be obtained at ~ 1.5 V vs RHE, where the OER still does not occur. Same result, with lower current density, can be obtained by using a methanol-containing electrolyte. This result demonstrates how GOR and MOR can be effective in lowering cell voltage for green hydrogen production with respect to classical water splitting. Then, stability tests demonstrated the durability of the electrode and the high Faradaic efficiency toward the formation of high value-added products.

4. Conclusions

The results demonstrate that TiO_2 nanotube electrodes functionalized with Ni and Co via electrodeposition are active toward the electrochemical oxidation of methanol and glycerol in alkaline media, showing also high durability. Therefore, alcohol electrooxidation could enable a reduction in electrolyzer cell voltage, allowing the simultaneous production of green hydrogen and value-added chemical products.

Acknowledgements

Some of the findings presented here are currently under patent application.

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LANAR CELL DESIGN FOR IMPROVED PERFORMANCE OF NaI–$AlCl_3$ EUTECTIC-BASED MOLTEN SODIUM BATTERIES – (C053)

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Keywords: Sodium-based batteries, Eutectic, Planar cell, NASICON

1. Introduction

The growing demand for reliable and cost-effective energy storage, driven by renewable energy integration, highlights the need for alternative battery technologies. While lithium-ion systems dominate, issues of resources availability and safety have stimulated interest in sodium-based solutions. Previous studies, including glass-housing batteries, have explored low-temperature molten sodium chemistries with promising performance[1]. Building upon this work, we introduce a planar battery containing NaI–$AlCl_3$ eutectic (NHB), able to reduce internal resistance by shortening the ionic path and enhancing interfacial contact with the NASICON solid electrolyte. This approach aims to improve low operating temperature and overall cell efficiency, representing a key novelty of this study.

2. Materials and Methods

A NaI–$AlCl_3$ eutectic (60:40) was used as molten electrolyte, with NASICON as solid electrolyte. The planar battery configuration is shown in Figure 1, highlighting the electrolyte, NASICON, and electrode layers. The design improves electrical contact and the accessibility of the cathodic material, reducing ionic path length. It also decreases the ratio of active to total internal volume, mitigating vapor loss. Tests were performed at 150 °C in an oven using a 162 mAh laboratory-scale cell.

3. Results and Discussion

Preliminary tests of the planar setup yielded encouraging results compared to previous batteries configurations. Improved electrical contact and enhanced accessibility of the cathodic material lead to efficient reversible electrochemical reactions. The planar configuration allows greater interaction between molten electrolyte and NASICON, overcoming the limitations of the former gravity-based contact. Vapor production, a known issue in these catholytes, is reduced due to the decreased ratio of active to total internal volume. Additionally, the new setup permits to expand the state-of-charge (SOC) range utilizing more active phase; previous constraints (7.5–29% SOC) were dictated by the old cell design, which prevented complete cycling.

Overall, these modifications demonstrate that cell architecture critically influences performance, efficiency, and operational stability, paving the way for future optimization through alternative eutectic compositions and further improvements in active mess utilization.



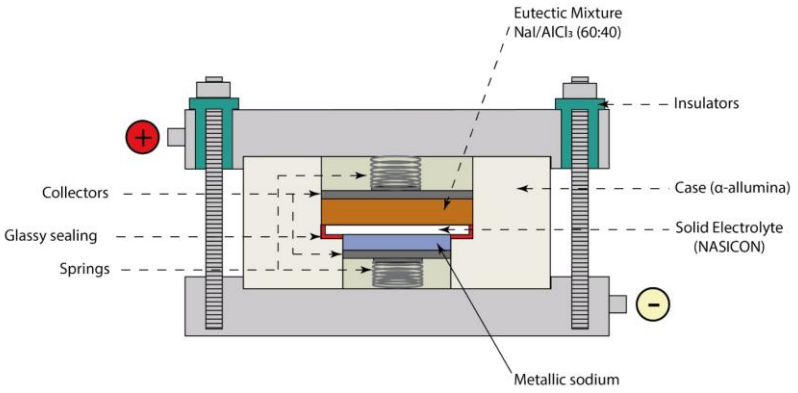


Figure 1 Sodium halide battery (planar configuration)

4. Conclusions

The planar NaI–$AlCl_3$ battery significantly enhances performance by improving electrical contact and cathode accessibility, reducing internal resistance and vapor loss. Expanded SOC and more efficient reversible reactions demonstrate the critical role of cell architecture. These results provide a foundation for further optimization of eutectic compositions and low-temperature sodium-based energy storage systems.

Acknowledgement

The authors gratefully acknowledge the University of Messina, in particular the XL Cycle of the Ph.D. Program in Engineering, for its institutional and scientific support.

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ADVANCING PLANAR NASICON BATTERIES THROUGH NI–FE COMPOSITES FOR IMPROVED PERFORMANCE UNDER MILD THERMAL CONDITIONS - (C054)

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Keywords: Mild temperature battery, NASICON, ZEBRA, Energy storage

1. Introduction

The development of solid-state sodium batteries capable of working under reduced thermal loads is increasingly relevant for improving energy efficiency and easing system integration in demanding environments. NASICON electrolytes remain among the most promising materials for this purpose, thanks to their high ionic conductivity and robust ceramic framework [1].

Nickel-based electrodes are widely employed in high-temperature sodium systems due to their reliable redox chemistry, but their cost motivates the exploration of partial substitution strategies. In particular, studies on sodium–metal halide batteries with Fe/Ni alloy cathodes have provided important insights into reaction mechanisms and the role of Fe in mixed Ni–Fe systems [2]. Building on this background, the present work investigates whether Ni–Fe composite electrodes can maintain reversible and cyclable behavior comparable to pure Ni when integrated into a planar NASICON-based solid-state battery operating under milder thermal conditions, while offering potential economic benefits due to reduced nickel content.

2. Materials and Methods

A planar NASICON solid electrolyte was fabricated and used as the core ceramic structure. Pure nickel and Ni–Fe (50:50 wt%) anodes were prepared as slurry-based coatings and deposited onto the NASICON substrate. After drying and stabilization, cells were assembled with suitable current collectors. Electrochemical behavior was assessed through galvanostatic charge–discharge tests at multiple C-rates and under reduced thermal conditions to evaluate rate capability, reversibility, and cycling stability of both electrode formulations.

3. Results and Discussion

Pure nickel electrodes exhibited stable and reliable electrochemical performance across the tested C-rates, particularly under higher-temperature conditions favorable to nickel kinetics. As the thermal load decreased, Ni electrodes displayed the expected rise in polarization and kinetic limitations yet retained good reversibility and sustained operation over the full range of investigated C-rates.

The Ni–Fe composite electrodes did not reach the C-rate capability of pure Ni, indicating that iron incorporation alters overall kinetic behavior—likely due to differences in redox activity and electronic transport. However, despite their reduced rate capability, Ni–Fe electrodes demonstrated fully reversible charge–discharge processes

and strong cycling stability. Importantly, they maintained reproducible behavior under milder thermal conditions, confirming that partial substitution of Ni with Fe does not compromise reversibility or long-term operability (Fig1). From an applications perspective, these findings are relevant for scenarios in which high-C-rate operation is not critical but cost efficiency is. Maintaining functional performance while reducing nickel consumption highlights Ni–Fe composites as a viable electrode option for cost-driven, NASICON-based solid-state battery designs.



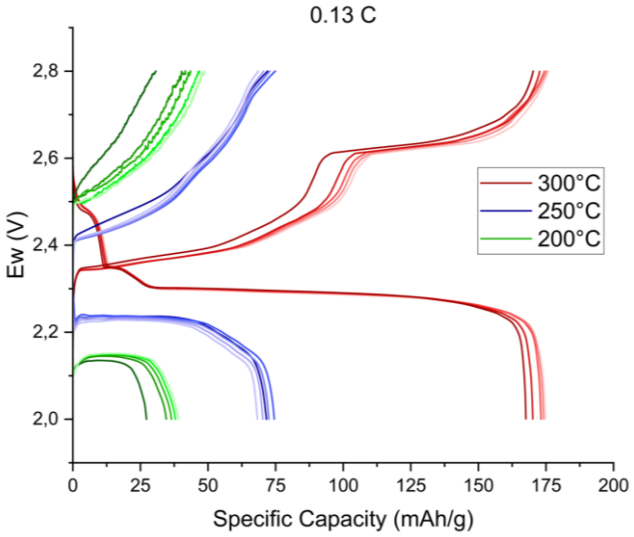


Figure 1. Charge–discharge cycling data for the 50% Ni / 50% Fe ZEBRA cell tested at 0.13 C, comparing performance metrics at operating temperatures of 200, 250, and 300 °C.

4. Conclusions

Planar NASICON-based cells showed stable operation under reduced thermal conditions using both Ni and Ni–Fe electrodes. While Ni–Fe composites do not match the C-rate capability of pure nickel, they maintain reversibility and stable cycling, supporting their use as a cost-efficient alternative when extreme rate performance is not essential. These findings encourage further development of economically optimized NASICON-based solid-state batteries designed for reduced thermal budgets and long-term reliability.

Acknowledgements

Authors from CNR-ITAE acknowledge the financial support from “Ministero dello Sviluppo Economico – Accordo di Programma MSE-CNR per la Ricerca del Sistema elettrico Nazionale”. (PTR 2025-2027)

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FIRST PRINCIPLES CALCULATIONS OF $SrTiO_3$ ENGINEERING WITH Bi BASED HETEROSTRUCTURES FOR EFFICIENT PHOTOSTIMULATED HYDROGEN PRODUCTION - (C056)

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Keywords: photostimulated hydrogen production, $SrTiO_3$, heterostructure, DFT calculations

1. Introduction

The urgent need for sustainable energy solutions has directed attention toward hydrogen (H_2) production via photocatalysis, harnessing sunlight as a renewable energy source. $SrTiO_3$ and $Bi_4Ti_3O_{12}$ are promising materials in this domain due to their excellent catalytic properties and structural versatility.

The layered $Bi_4Ti_3O_{12}$ structure, composed of alternating pseudo-perovskite $(Bi_2Ti_3O_{10})^{2-}$ and $(Bi_2O_2)^{2+}$ layers, promotes the growth of this material in a favourable two-dimensional (2D) morphology. In contrast, the symmetrical crystal structure of $SrTiO_3$ does not facilitate the spontaneous formation of 2D $SrTiO_3$ nanostructures.

However, due to the structural similarity between $SrTiO_3$ and the pseudo-perovskite units of $Bi_4Ti_3O_{12}$, combined with favorable dissolution and transformation chemistries under hydrothermal conditions, $Bi_4Ti_3O_{12}$ template nanoplatelets can gradually transform into $SrTiO_3$ nanoplatelets. This occurs through a process of template dissolution and epitaxial $SrTiO_3$ growth, resulting in 2D/2D epitaxial $SrTiO_3/Bi_4Ti_3O_{12}$ nano-heterostructures at the intermediate stage and $SrTiO_3$ nanoplatelets at the final stage of transformation [1,2]. Some bismuth remains incorporated into the $SrTiO_3$ or becomes trapped on its surface. The most typical and always present is the monoatomic bismuth oxide (BiO) layer, which extends across the middle and along every transformed $SrTiO_3$ platelet. By carefully controlling the transformation process, the material's photocatalytic performance can be significantly enhanced.

2. Materials and Methods

In this study we investigated the electronic and geometric properties of BiO layer in $SrTiO_3$ and $SrTiO_3/Bi_3Ti_4O_{12}$ heterostructure using first principles DFT calculations. We employed state of the art hybrid DFT calculations and linear combination of Gaussian orbitals basis sets as implemented in Crystal23 software [3,4].

3. Results and Discussion

The calculated $SrTiO_3$ band gap is 3.2 eV, while $Bi_3Ti_4O_{12}$ – 3.8 eV. Figure 1 shows the density of states of their heterostructure. As one can see, the band gap of the latter is 2 eV, very suitable for the sun light use in photostimulated hydrogen production. The



top of the valence band is produced by SrO layer while the bottom of the conduction band – BiO layer, which is type II heterostructure.

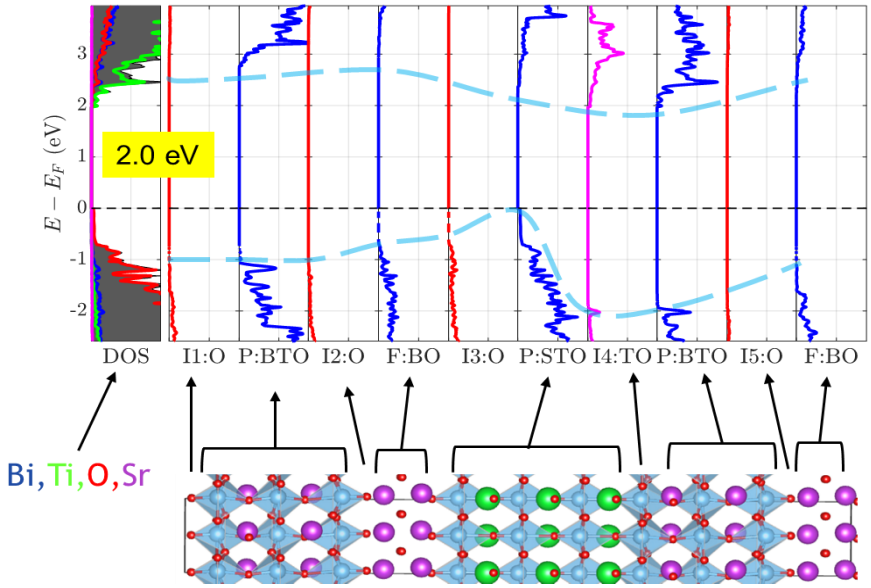


Figure 1. The projection of the density of states onto different planes of the $SrTiO_3/Bi_4Ti_3O_{12}$ interface.

4. Conclusions

We have demonstrated the band gap decrease with Bi containing layer incorporation into $SrTiO_3$ resulting in either $SrTiO_3/Bi_4Ti_3O_{12}$ heterostructure or BiO monolayer in $SrTiO_3$ models. In the latter case, we distinguish either Bi or Ti, Sr vacancy compensation mechanism. Thus, this system is promising for the sun light hydrogen production.

Acknowledgements

The GRIPHUS project, co-funded by Regione Calabria, the Ministry of Higher Education, Science and Innovation of Slovenia, and the Latvian Council of Science within the framework of the M-Era.Net Call 2024, is gratefully acknowledged for co-funding this work.

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HIGH ACTIVE-MASS FREE-STANDING $Na_4MnCr(PO_4)_3$/CNF CATHODES FOR SODIUM-ION BATTERIES - (C057)

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Keywords: NASICON cathode, free-standing electrode, carbon nanofibers, sodium-ion batteries.

1. Introduction

Sodium-ion batteries (SIBs) are emerging as a sustainable alternative to lithium-ion systems for large-scale energy storage [1], and NASICON-type phosphates [2] are attractive cathodes thanks to their robust three-dimensional framework and high structural stability. In the previous ICSET contribution, freestanding $Na_4MnCr(PO_4)_3$/CNF electrodes with 40 wt% active material were reported. However, the low active mass fraction can increase the capacitive contribution of the carbon matrix, hindering an accurate evaluation of the intrinsic electrochemical behavior of the NASICON phase. This work continues the previous study and aims to develop free-standing $Na_4MnCr(PO_4)_3$/CNF cathodes with increased active material loading while preserving flexibility and mechanical integrity.

2. Materials and Methods

Two fabrication strategies were investigated: a one-step route, in which CNFs and $Na_4MnCr(PO_4)_3$ were simultaneously formed by electrospinning, and a two-step route, in which CNF membranes were first prepared by electrospinning a PAN solution (stabilization at 270 °C in air and carbonization at 900 °C in N_2), and subsequently impregnated with $Na_4MnCr(PO_4)_3$ precursors by dip-coating. The materials were characterized by XRD, SEM and TGA, and electrochemically tested in half cells by CV and galvanostatic test.

3. Results and Discussion

The two-step fabrication strategy enabled the preparation of free-standing $Na_4MnCr(PO_4)_3$/CNF electrodes with an active material loading of about 70 wt%, as confirmed by thermogravimetric analysis in Fig 1a. X-ray diffraction patterns (Fig. 1b) evidenced the formation of the rhombohedral NASICON structure, while electron microscopy (Fig.1c) revealed a homogeneous distribution of $Na_4MnCr(PO_4)_3$ nanocrystals along the conductive CNF network, preserving the interconnected fibrous architecture required for binder-free operation. Electrochemical tests performed in half-cell configuration in the 1.5–4.5 V vs. Na^+/Na range showed that the high-loading composite delivers a specific discharge capacity higher than 125 mAh g^{-1} at 0.1C (Fig. 2a). In addition, the electrode exhibits a capacity retention exceeding 80% after 100 charge–discharge cycles and a coulombic efficiency above 90% (Fig. 2b), demonstrating good reversibility and structural stability despite the significantly increased active material content. These results represent a clear improvement with respect to the previously reported 40 wt% composites.

and confirm that the two-step approach is crucial to achieve high active mass fractions without compromising electrochemical performance.



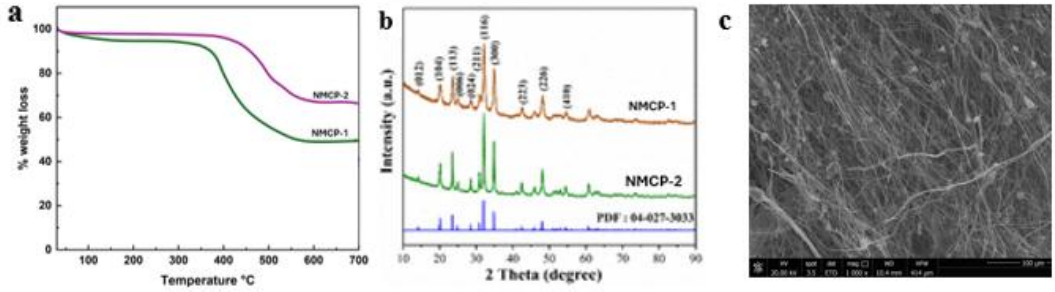


Figure 1. (a) TGA curves of $Na_4MnCr(PO_4)_3$/CNF composites. (b) XRD patterns confirming the NASICON phase. (c) SEM image of the free-standing $Na_4MnCr(PO_4)_3$/CNF nanofibrous electrode.

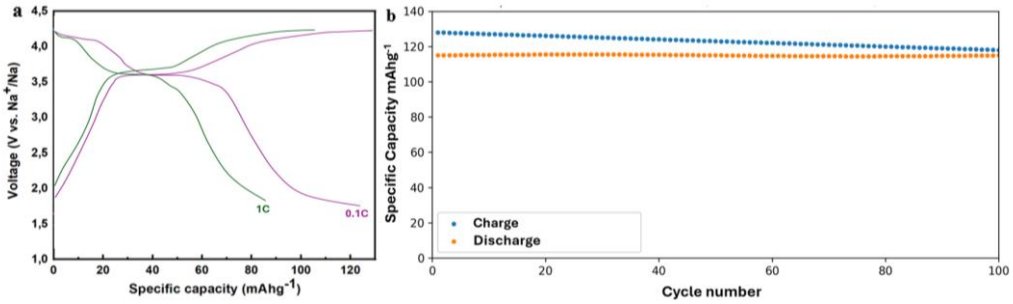


Figure 2. (a) Charge–discharge profiles of the $Na_4MnCr(PO_4)_3$/CNF electrode at different C-rates. (b) Cycling performance showing charge and discharge specific capacities over 100 cycles.

4. Conclusions

A two-step fabrication strategy was successfully adopted to produce flexible and free-standing $Na_4MnCr(PO_4)_3$/CNF cathodes with an active material loading of about 70 wt%. The optimized electrodes achieve specific capacities higher than 125 mAh g^{-1} at 1C, capacity retention above 70% after 100 cycles and coulombic efficiency higher than 90%. The proposed architecture represents an effective route to scale up NASICON-based self-supporting cathodes for sustainable sodium-ion battery technologies.

Acknowledgements

This work was supported by the Italian Ministry for the Environment and Energy Security (MASE) and CNR within the "Accordo di Programma MASE–CNR per la Ricerca del Sistema Elettrico Nazionale" (PTR 2025–2027).

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DOUBLE SUBSTITUED Co-FREE PEROVSKITE OXIDES FOR REVERSIBLE SOLID OXIDE CELLS (RSOCs) - (C058)

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Keywords: Perovskite oxides, B-site substitution, SOEC, CO_2 conversion, reversible solid oxide cell (RSOC)

1. Introduction

High-temperature CO_2 electrolysis in solid oxide electrochemical cells offers one of the most efficient routes for carbon dioxide conversion. The emergence of CO:CO_2 reversible solid oxide cells (RSOCs) enhances system efficiency promoting integration with CO_2- and CO-rich industrial exhaust streams. However, reversible operation imposes stringent requirements on electrode materials, which must combine high catalytic activity, redox stability, and long-term durability under a wide range of oxygen partial pressures. The effect of 20 mol% B-site substitution in $La_{0.6}Sr_{0.4}Fe_{0.6}Mn_{0.4}O_{3-\delta}$ (LSFM) was explored to enhance electrocatalytic performance for reversible solid oxide cell (RSOC) electrodes. Specifically, $La_{0.6}Sr_{0.4}Fe_{0.6}Mn_{0.2}Cu_{0.2}O_{3-\delta}$ (LSFMC) and $La_{0.6}Sr_{0.4}Fe_{0.6}Mn_{0.2}Ni_{0.2}O_{3-\delta}$ (LSFMN) single phases were synthesized and characterized as air and fuel electrodes, respectively. A quasi-symmetric LSGM-supported cell with LSFMN at the fuel side and LSFMC at the air side demonstrated remarkable performance in both CO-SOFC and CO_2-SOEC modes.

2. Materials and Methods

Doped lanthanum ferrites of formula LSFM, LSFMN and LSFMC were prepared by auto-combustion of dry gel obtained from a solution of the corresponding nitrates into citric acid solution. Phase purity, lattice symmetry, and unit-cell parameters were determined by powder X-ray diffraction (XRPD). A field emission scanning electron (FE-SEM) microscope Carl Zeiss FE-SEM, SUPRA™ 35 and a Transmission Electron Microscope (TEM) FEI Tecnai G2 F20 were used for morphological analysis on as prepared and reduced samples. Electrochemical measurements were carried out on $La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ (LSGM) electrolyte-supported cells. Cell tests were performed on a lab-scale station, using a PARSTAT 2273 potentiostat-galvanostat/EIS analyzer at 850 °C, with the air side exposed to static air and the fuel side exposed to constant flux of 100 $cm^3 \cdot min^{-1}$ of the inlet gas, depending on the tests (pure H_2, pure CO_2 and 50:50 CO:CO_2).

3. Results and Discussion

LSGM-based semi-symmetric cell was fabricated, with LSFMC electrode at the air side and LSFMN electrode at fuel side (Fig. 1). The semi-symmetric LSFMN/LSFMC cell presents a maximum power density (MPD) of 371 $mW \cdot cm^{-2}$ and a current density of -0.94 $A \cdot cm^{-2}$ at 1.5 V. As reversible SOCs in a 50:50 CO:CO_2 gas mixture, the semi-symmetric LSFMN/LSFMC cell achievied a MPD of 168 $mW \cdot cm^{-2}$ in SOFC mode and a current density of -0.69 $A \cdot cm^{-2}$ at 1.5V in SOEC mode, The electrochemical results confirm that the combination of the high catalytic activity of exsolved Ni-based nanoparticles at the fuel side and the enhanced oxygen reactions activity introduced by Cu-substitution at the air side is a promising strategy to improve cell performance. A long-term reversible stability test was carried out in a 50:50 CO:CO_2 gas mixture. The current density was monitored during several SOFC/SOEC cycles at different voltages (0.7 V and 1.2 V, respectively) for up to 150 h operation. Most current density loss occurred during the first of operation can be attributed to initial system equilibration. After this point, the device shows great stability during over 100 h operation, with a total current density loss of 6% and 12% in SOFC and SOEC mode, respectively. To assess morphological stability after operation, a post-mortem SEM-EDX analysis of the cell has been performed. From the micrograph of



spent LSFMN fuel electrode, the perovskite results not damaged and still covered by clearly visible and non-coarsened nanoparticles with an average dimension < 100 nm. EDX analysis

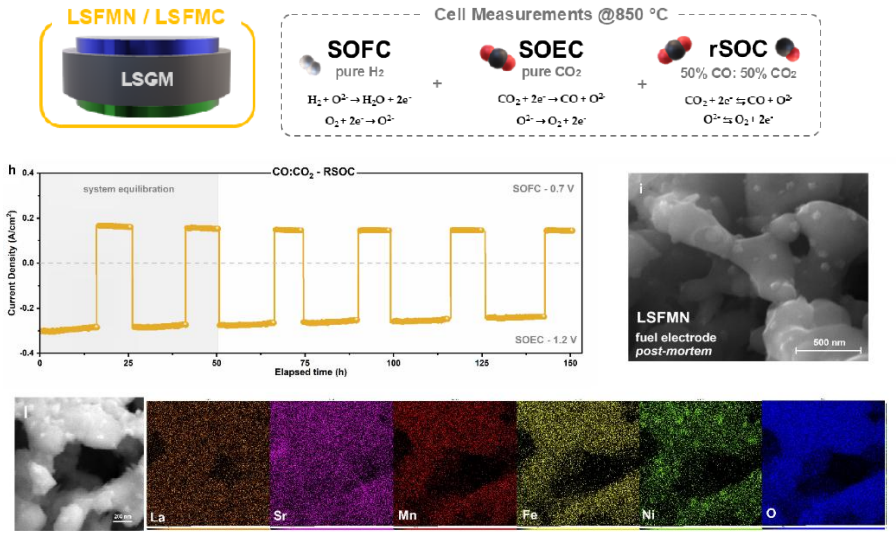


Figure 1 - Cell Tests: Scheme of cells architectures (LSFMN/LSFMC) and electrochemical testing carried out at 850 °C in different operational modes and gas-inlet compositions (H_2-SOFC, CO_2-SOEC, CO:CO_2 RSOC); Long-term reversible stability in CO:CO_2 up to 150 h; SEM and EDX post-mortem analysis of spent LSFMN fuel electrode after long-term stability test.

4. Conclusions

A quasi-symmetric LSGM-supported cell employing LSFMN at the fuel electrode and LSFMC at the air electrode delivers high performance and stable operation in both CO-SOFC and CO_2-SOEC modes, maintaining reversibility for over 150 h without detectable degradation. Overall, exsolution-engineered Mn-stabilized ferrites are established as a robust, cobalt-free electrode platform for RSOCs, highlighting metal exsolution as a powerful tool to simultaneously achieve high catalytic activity, redox resilience, and long-term durability in reversible CO:CO_2 electrochemical conversion.

Acknowledgements

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INTEGRATED SYSTEM ANALYSIS OF BIOGAS-TO-METHANOL PRODUCTION WITH UPSTREAM CO_2 CAPTURE BY CALCIUM LOOPING AND CERIA-BASED CHEMICAL LOOPING SYNGAS GENERATION - (C060)

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Keywords: Calcium looping, Chemical looping, Biogas, Methanol, Carbon Capture and Utilisation.

1. Introduction

Renewable methanol from biogas is attracting attention as a low-carbon fuel/chemical, but most published flowsheets rely on catalytic reforming with downstream methanol synthesis and typically require CO_2 separation units and fired heat supply. Recent techno-economic studies show that placing CO_2 removal upstream of reforming improves carbon and fuel efficiencies, yet still vents significant biogenic CO_2 and adds process complexity [1]. Here we propose a four-reactor **Ca-looping + ceria chemical-looping** front-end that directly feeds a MeOH reactor, aiming at high efficiency and low specific emissions without extra biogas firing.

2. Materials and Methods

A steady-state process model couples: CaO carbonator/calciner for CO_2 management and a ceria-based CLMR reducer/steam-oxidiser to generate a combined syngas stream (overall $H_2/CO \approx 3$). The syngas is fed to methanol synthesis at 250 °C and 100 bar. Heat integration is assessed at system level; auxiliary electricity includes multistage compression and a calciner vacuum pump. A sensitivity analysis was performed in the four main thermochemical reactor and operating conditions of the ethanol synthesis section.

3. Results and Discussion

At the selected operating point, **1.67 kmol/h biogas** (1 kmol/h CH_4; 0.67 kmol/h CO_2) is converted to **0.842 kmol/h methanol** with **98.33% purity** and **89% CH_4 conversion**. CO_2 is largely removed upstream (**0.64 kmol/h**) with a limited residual biogenic release (**0.19 kmol/h**), corresponding to **0.3 $kgCO_2/kgMeOH$**. The process requires **223.2 kW** of fuel input and delivers **149.3 kW** as MeOH LHV; auxiliary electricity totals **16.8 kW**, giving **62% electric efficiency** and **86% global efficiency** when the **57.3 kW cold utility** is credited. No additional biogas firing is needed (biogas to combustion = 0); the thermal balance is closed by recovering heat from unreacted gases leaving the MeOH section. The biogas mole flow rate was chosen to normalise all the parameters and KPI to 1 kmol/h of methane in input to the complete system.

Compared with conventional biogas-to-MeOH schemes based on fired reforming and solvent CO_2 removal, which report carbon efficiencies around ~50% and biogenic CO_2 emissions on the order of ~1.2 $kgCO_2/kgMeOH$ in representative base cases, the proposed looping front-end achieves **similar carbon efficiency (50%)** with markedly lower specific biogenic CO_2 emissions in this operating point.



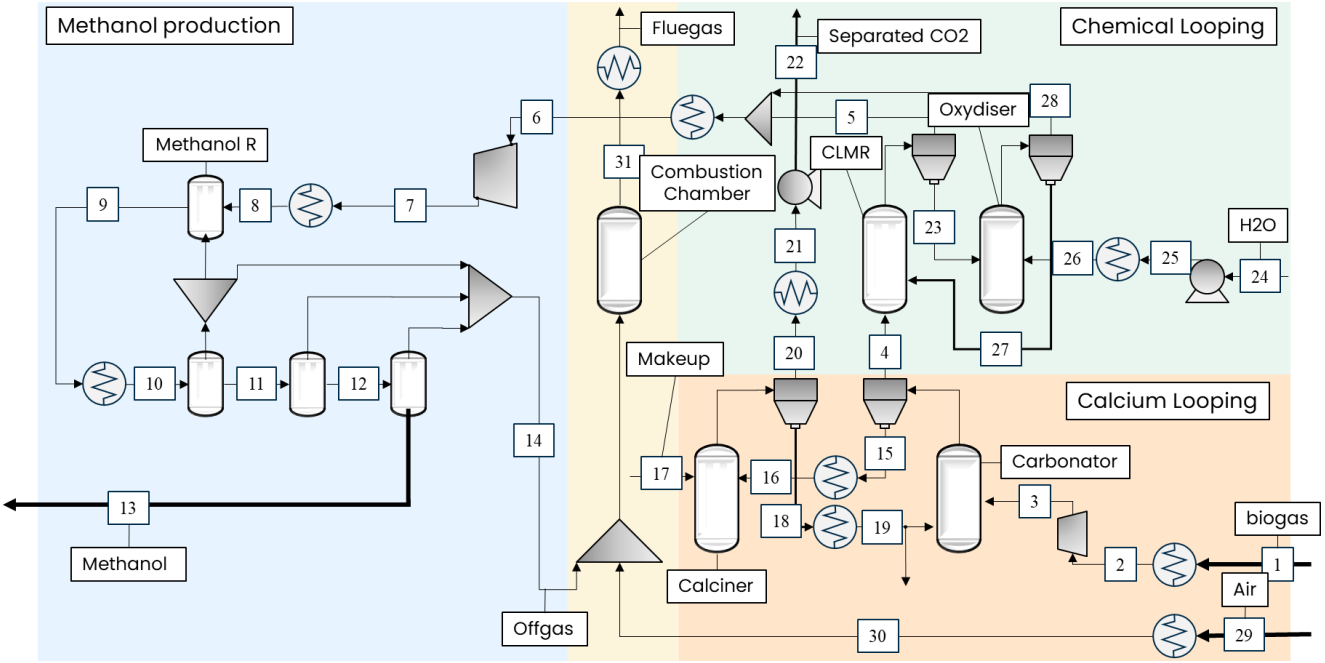


Figure. Biogas to methanol pathway through a Calcium Looping CO2 capture and ceria based Chemical Looping syngas production

4. Conclusions

An integrated Ca-looping/ceria chemical-looping front-end enables biogas-to-methanol production with high conversion efficiency and strongly reduced specific biogenic CO_2 emissions, while avoiding additional biogas firing through heat recovery from the MeOH section. Future work will develop kinetic reactor models and preliminary reactor designs for the CaL and ceria looping units, and will extend the analysis to a full techno-economic assessment to quantify the resulting levelised methanol cost.

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DENSITY FUNCTIONAL THEORY CALCULATIONS ON G-C3N4/SRTIO3 HETEROSTRUCTURE - (C061)

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Keywords: graphitic carbon nitride, perovskite, heterostructure, CO_2, DFT

1. Introduction

Catalytic properties are known to be dependent to high extent on the atomic structure and chemical bonding characteristics of a material. In particular, the mechanism of photocatalytic reaction is governed by these properties when two materials are combined in a heterostructure. Graphitic carbon nitride (g-C_3N_4) plays an important role due to its band gap value of 2.7 eV [1], and its combination with a perovskite system such as $SrTiO_3$ is considered highly promising for photocatalytic applications. However, despite the critical role of atomic structure and chemical bonding in determining the behavior of adsorbed molecules at the surface, a thorough analysis of these aspects is still lacking.

2. Materials and Methods

The density functional theory (DFT) calculations were performed using the plane wave code VASP6 to study the electronic and atomic structure properties and CO_2 behavior on the g-C_3N_4/$SrTiO_3$ heterostructure within a slab model. The DFT calculations used a PBE functional and van der Waals interaction corrections using the D3 scheme. The main emphasis is put on band structure analysis and CO_2 adsorption sites. Initial 2D atomic structure of g-C_3N_4 was taken from experimental observation [2] and, thus, was a tri-s-triazine-based polymeric structure and contained hydrogen atoms in a small amount. In the present calculations the number of g-C_3N_4 and $SrTiO_3$ layers was varied to clarify the role of inter- and intra-layer interactions on the resulting properties, for example, 1-layer-g-C_3N_4/ $SrTiO_3$ model and 2-layer-g-C_3N_4/$SrTiO_3$ models.

3. Results and Discussion

The present DFT calculations have considered a heterostructure of g-C_3N_4/$SrTiO_3$. The focus is laid on its electronic, chemical bonding and atomic structure properties without and with adsorption of CO_2 molecule. As of the system without the CO_2 molecule, the calculated band structure, density of states and chemical bonding properties are thoroughly analyzed depending on the number of layers on both sides of the heterostructure. We emphasize differences in the atomic structure relaxation in the comparison with the one-layer model and analyze deeply the chemical bond formations in such a model from effective atomic charges and electronic charge distributions. Notice that the two layers of g-C_3N_4 are shifted with respect to each other in accordance with a recent experimental work [2]. The TiO_2 terminated surface is sufficiently more preferential as the total energy difference between the two terminations, namely SrO and TiO_2, is approx. 1.18 eV/cell. An indirect band gap of 1.03-1.09 eV is found by the PBE functional depending on the model. One layer of g-C_3N_4 lying on the TiO_2-terminated surface of $SrTiO_3$ has a “wave-like” shape [3]. In this case strong N-H bonds (of typically 1.04 Å bond length which is also in line with [2]) have an impact on the obtained atomic structure in such a way that the distances between the layers are shortened (Figure) in their positions in both directions: the neighboring g-C_3N_4 layer and TiO_2 layer. We find the shortest N-N distance between N atoms in the two layers 3 Å and the shortest distance between H and O in the TiO_2 layer 2.14 Å. It would potentially affect catalytic properties of g-C_3N_4/$SrTiO_3$ heterostructures.



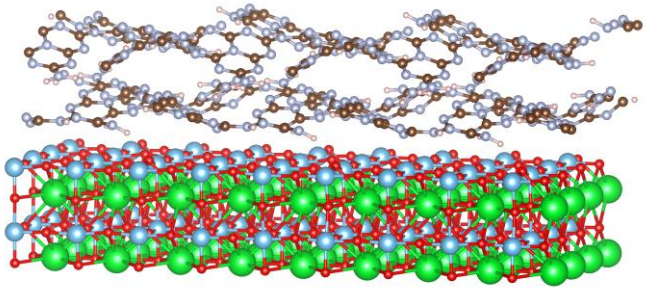


Figure. Example of fully relaxed 2-layer-*g*-C_3N_4/$SrTiO_3$ heterostructure. TiO_2-terminated surface of $SrTiO_3$ is considered. Green: Sr, blue: Ti, red: O, white: H, bright grey: N, yellow: C.

4. Conclusions

The *g*-C_3N_4/$SrTiO_3$ heterostructure was investigated by the DFT calculations based on several structural models to address its chemical bonding and atomic structure properties. In particular, the number of layers in both *g*-C_3N_4 and $SrTiO_3$ was varied to analyze the role of existing inter- and intra-layer interactions for such properties. Thus, the DFT calculations demonstrate that the 2-layer-*g*-C_3N_4/$SrTiO_3$ model is a specially relevant for accurately describing the heterostructure, owing to strong N-H bonds and induced distortions of atomic structure in both *g*-C_3N_4 and $SrTiO_3$.

Acknowledgements

The GRIPHUS project, co-funded by Regione Calabria, the Ministry of Higher Education, Science and Innovation of Slovenia, and the Latvian Council of Science within the framework of the M-Era.Net Call 2024, is gratefully acknowledged for co-funding this work. The authors thank Dr. Marjeta Maček Kržmanc for stimulating discussions.

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PERFORMANCE AND DURABILITY IMPROVEMENT OF LSCF ELECTRODE FOR SOLID OXIDE ELECTROLYSIS - (C063)

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At the next stage of technological development, solid oxide electrolysis cells (SOECs) are expected to operate at current densities of around -1.5 A.cm^{-2} while maintaining degradation rates below 0.5% per 1000 hours under relevant operating conditions [1].The state-of-the-art material for oxygen electrode in solid oxide cells (SOCs) is $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ (LSCF), but its performance remains limited, and more importantly it suffers from significant degradation, which are mainly attributed to the electrode material decomposition occurring in operation [2]. To improve the cell performance, a conventional $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta} - Ce_{0.8}Gd_{0.2}O_{2-\delta}$ (LSCF-CGO) composite electrode was infiltrated by praseodymium oxide. The polarization resistance (Rp) of the infiltrated electrode measured on symmetrical cell was substantially improved with respect to the LSCF-CGO composite (Figure 1a). Furthermore, electrochemical characterizations conducted of the infiltrated complete cells have also revealed high initial performances at 750°C (-1A/cm² @1.24V @12 NmL/min/cm^2 with H_2O/H_2=90/10). To improve the durability of LSCF, it has recently been proposed to replace LSCF by High Entropy Oxides (HEOs), which are expected to be more stable during operation [3]. In this context, Mn-doped LSCF (LSMCF) is a promising HEO material that exhibit good performances and stability (Figure 1b) [3]. In this study, Hybrid Density Functional Theory (DFT) calculations were coupled to a thermodynamic defect model which permitted to quantify the decomposition rate of LSCF due to Cr-poisoning. This decomposition is shown to be thermodynamically highly favorable at typical SOCs operating temperatures even at partial pressures of CrO_3 as low as 10-10 atm. This model was subsequently used to quantify the decomposition rate of HEO-LSMCF. LSMCF powder has been successfully synthesized without secondary phases, and the porous electrodes have been manufactured by screen printing. The electrochemical characterization of this LSMCF electrode is ongoing.

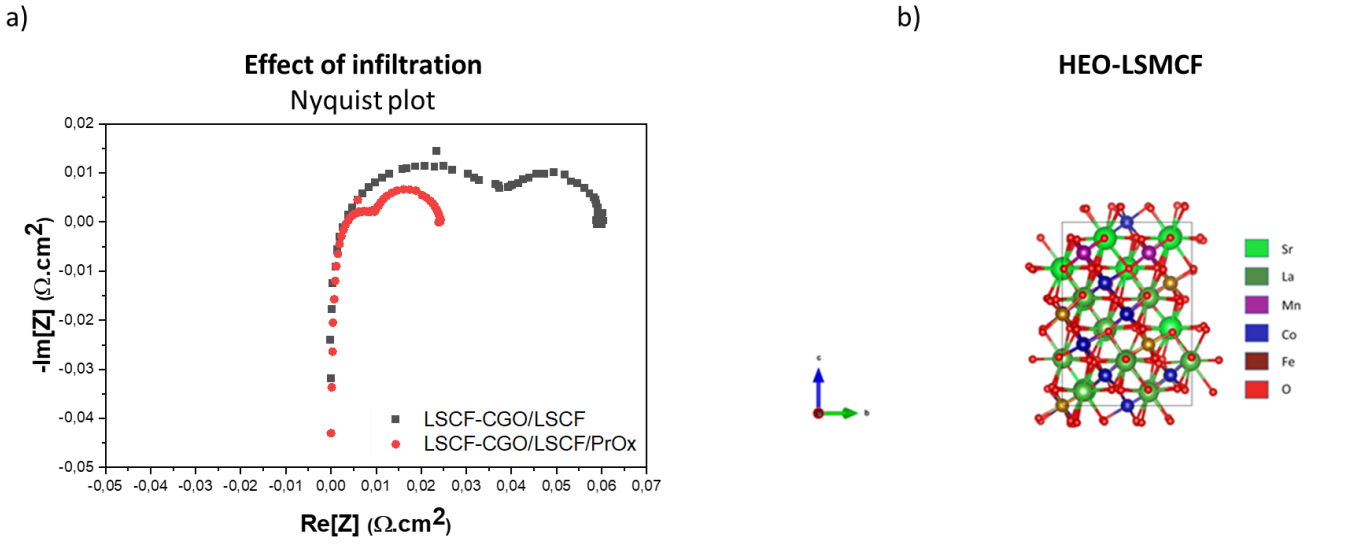


Figure 3: a) Nyquist plots at 750°C PO_2=0.21 atm; b) atomic structure of HEO-LSMCF



Acknowledgements

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NEW ENVIRONMENTALLY FRIENDLY MECHANOCHEMICAL SYNTHESIS OF Cu-BASED CATALYSTS FOR E-METHANOL PRODUCTION - (C064)

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Keywords: Catalysts, Mechanochemical synthesis, Green Hydrogen, E-methanol, CO_2.

1. Introduction

The increasing atmospheric concentration of CO_2 caused by the use of fossil fuels has become a primary issue. Converting CO_2 and green H_2 into synthetic fuels like E-methanol is a promising solution for recovering CO_2 and storing renewable energy in chemical form. Moreover, E-fuels can be used directly in the existing infrastructure (storage, transport and use) [1]. E-methanol production requires redox catalysts with high activity [2]. The conventional synthesis of these materials usually involves several long steps with high energy and water consumption; in contrast, mechanochemical synthesis can be faster and greener [3]. In this work a series of promising Cu/Zn/Al (CZA) materials for methanol synthesis were prepared with an innovative, fast and solvent-free mechanochemical method.

2. Materials and Methods

The catalysts were prepared with a new solvent-free mechanochemical method, using an MM 500 Control ball mill (Retsch) equipped with stainless steel jars and balls. In one series, metal nitrates were milled at 30 Hz with NaOH for different times (10-60 min). Another series was prepared milling the nitrates with NaOH and Na_2CO_3 (ex-LDH) at 20 Hz for 10 and 30 min. All the samples were washed and calcined at 500 °C, then characterized with ICP, XRD, N_2 physisorption, and SEM and tested for methanol production at 250 °C and 3 MPa.

3. Results and Discussion

All the prepared materials present interesting XRD patterns: the materials prepared with NaOH show the formation of both CuO and ZnO crystalline structures, with only marginal differences in the crystallinity of ZnO between the samples prepared at different duration time. However, only for milling time higher than 30 min the solid obtained before the calcination is sufficiently homogeneous. The materials prepared with NaOH and Na_2CO_3 show, before the calcination, the typical pattern of hydrotalcite-like materials (LDH), whereas after the calcination both CuO and ZnO crystalline phases are present, with smaller crystallites than the previous series. Also in this case, for different milling times the differences are negligible, but the reproduction of the material was possible only for the 30 min treatment (Fig 1a). The materials of the first series show type II isotherms (Fig 2b) typical of microporous solids and possess poor textural properties (S_{BET} ca. 15 m^2g^{-1}, V_p ca. 0.04 cm^3g^{-1}); on the other hand, the ex-LDH oxides of the second series show complex type IV+II isotherms (Fig 2b) which indicates the presence of both meso- and macropores. In this case the textural properties are better (S_{BET} ca. 50 m^2g^{-1}, V_p ca. 0.31 cm^3g^{-1}) and very similar to those of analogue materials obtained with the conventional coprecipitation synthesis of LDHs. The best materials of each series were tested for the CO_2 hydrogenation into E-methanol, using a fixed bed tubular reactor filled with the catalysts and α-Al_2O_3, at 250 °C and 3 MPa, with a GHSV of 24000 NmL g_{cat}^{-1} h^{-1} for 15 h. The catalysts prepared with only NaOH showed limited CO_2 conversion (6.6 %) and average methanol selectivity (18.1 %), with a space-time yield (STY) of 90.7 mg_{MeOH} g^{-1} h^{-1}. On the contrary, the best ex-LDH catalysts



show interesting CO_2 conversion (11.5 and 14.1 %) and promising methanol selectivity (17.2 and 28.9 %), showing noteworthy STY (150.7 and 306.6 mg_{MeOH} g^{-1} h^{-1}), in line with the performance of similar materials prepared with the conventional methods.

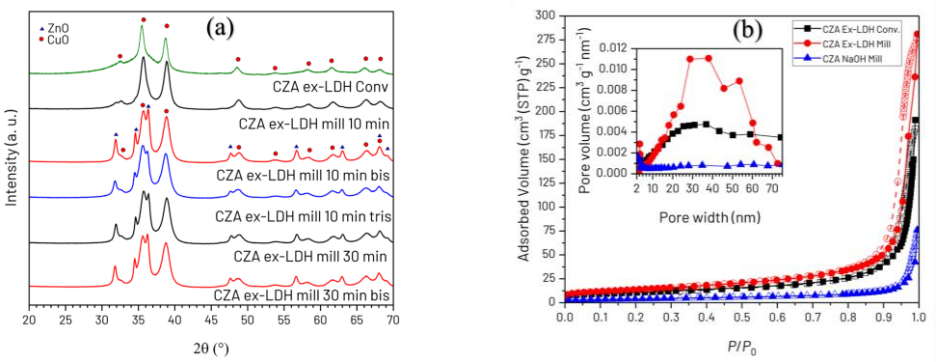


Figure 1 – Characterization of the catalysts prepared with the mechanochemical methods and the conventional one for comparison: XRD patterns (a) and N_2 physisorption (b)

4. Conclusions

The mechanochemical method proposed in this work allowed the efficient synthesis of a series of active catalysts for E-methanol production, with limited power and water consumption (room temperature and solvent-free) and strongly reducing the process duration (from days to hours). The material prepared with the mechanochemical LDHs synthesis method showed physical-chemical and catalytic properties very similar to those of the analogous materials prepared with the conventional coprecipitation synthesis.

Acknowledgements

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ENGINEERING 2D SRTIO₃ NANOSTRUCTURES FOR ENHANCED PHOTOCATALYTIC H₂ EVOLUTION THROUGH AURIVILLIUS-PHASE Bi₄Ti₃O₁₂ TRANSFORMATION - (C071)

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Keywords: $SrTiO_3$ nanoplatelets, hydrothermal transformation, photocatalytic H_2 generation, Aurivillius phase $Bi_4Ti_3O_{12}$

1. Introduction

Two-dimensional (2D) nanostructures are highly attractive for photocatalysis due to their high density of active surface sites and efficient transport of photoinduced charge carriers. Although $SrTiO_3$ has a relatively wide band gap (3.2 eV), it is a well-studied photocatalyst for H_2 evolution because of its sufficiently negative conduction band potential (−0.8 V vs. NHE) [1]. However, its highly symmetric crystal structure favours the formation of three-dimensional, cube-like particles rather than 2D morphologies. We demonstrate, for the first time, that 2D $SrTiO_3$ nanostructures can be synthesised via the topochemical transformation of $Bi_4Ti_3O_{12}$ nanoplatelets under alkaline hydrothermal conditions. Our additional aim is to explore synthesis strategies for controlling the functional properties of $SrTiO_3$ nanoplatelets for photocatalytic H_2 evolution.

2. Materials and Methods

Template $Bi_4Ti_3O_{12}$ nanoplatelets were synthesised from well-mixed Bi_2O_3 and TiO_2 nanopowders in molten NaCl/KCl salt at 800°C [2,3]. After separation from the salt by water washing, the $Bi_4Ti_3O_{12}$ nanoplatelets were used as the template for the transformation into $SrTiO_3$ nanoplatelets under alkaline hydrothermal conditions (6M NaOH, 200°C, Sr/Ti=12-15). XRD, XPS, SEM, and STEM were the main characterisation techniques for structural, chemical and morphological characterisation of the product. Photocatalytic H_2 evolution was tested without the addition of any noble metal co-catalysts in water/methanol (75/25) under Xenon irradiation, and H_2 was quantified by gas chromatography.

3. Results and Discussion

The transformation of $Bi_4Ti_3O_{12}$ template nanoplatelets into 2D $SrTiO_3$ nanostructures under alkaline hydrothermal conditions proceeds via template dissolution followed by epitaxial growth of $SrTiO_3$ [2,3]. $SrTiO_3$ nanoplatelets with varying surface roughness were prepared by systematically varying experimental parameters such as the $Bi_4Ti_3O_{12}$ template size, strontium excess (Sr/Ti molar ratio), and the temperature of the initial NaOH solution.

The transformation of smaller template nanoplatelets, combined with pretreatment in warm NaOH and higher Sr excess (Sr/Ti = 15), resulted in rougher $SrTiO_3$ nanoplatelets with a higher BET surface area (61 m^2/g). In contrast, using larger templates, lower Sr excess ($Sr/Ti \leq 12$), and no pretreatment produced smoother $SrTiO_3$ nanoplatelets with a BET surface area of 11 m^2/g. Photocatalytic testing revealed that high-surface-area platelets exhibited approximately 27 times higher H_2 evolution rates compared to their smooth counterparts (Fig. 1). Combined STEM and ex-situ XPS analyses indicated that the enhanced H_2 evolution performance correlates with surface-trapped bismuth single atoms, which act as non-noble-metal co-catalysts for photocatalytic hydrogen evolution.

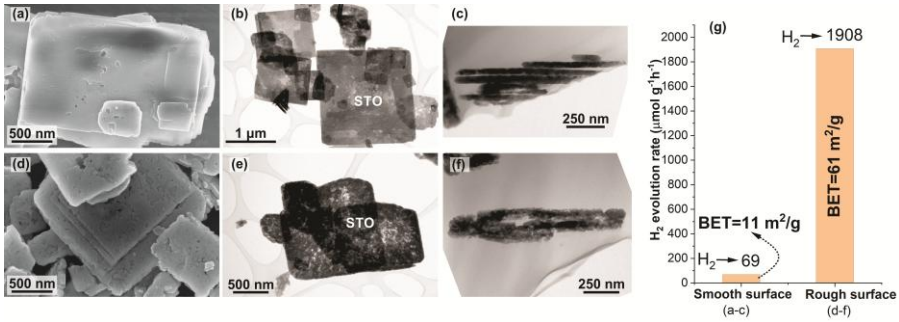


Figure 1. (a, d) SEM and (b, c, e, f) STEM micrographs of the representative smooth (a-c) and rough (d-f) $SrTiO_3$ nanoplatelets. (g) Comparison of H_2 evolution rates and BET surface area values for both types of 2D $SrTiO_3$.

4. Conclusions

Controlling the experimental parameters of the $Bi_4Ti_3O_{12}$-to-$SrTiO_3$ hydrothermal transformation enables precise tuning of surface roughness, stabilisation of surface-trapped Bi single atoms, and modulation of the photocatalytic properties of 2D $SrTiO_3$ nanostructures. The demonstrated transformation provides a versatile platform for engineering other $Bi_4Ti_3O_{12}$-derived 2D $ATiO_3$ perovskites with broad application potential in piezocatalysis, pyrocatalysis, dual-functional photocatalysis, and related fields.

Acknowledgements

The GRIPHUS project, co-funded by Regione Calabria, the Ministry of Higher Education, Science and Innovation of Slovenia, and the Latvian Council of Science within the framework of the M-Era.Net Call 2024, is gratefully acknowledged for co-funding this work.

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ELECTRIFIED MEMBRANE REACTOR FOR NH_3 DECOMPOSITION: COMBINING H_2 SCAVENGING AND EFFECTIVE HEAT SUPPLY - (C072)

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Keywords: Hydrogen, Ammonia, Electrified reactor, Membrane reactor.

1. Introduction

Ammonia is one of the most promising H_2 carriers. The two main challenges for the scale-up of NH_3 decomposition are achieving effective heat transfer and addressing the strong H_2 inhibition that affects the best-performing Ru-based catalysts [1]. To address both challenges, we propose the design of a novel electrified membrane reactor (e-MR): the introduction of a Pd-Ag membrane dramatically increases the reaction rate by removing H_2 from the catalyst surface, and electrification ensures better coupling between heat supply and demand, approaching the ideal performance of an isothermal reactor. As a result, it is possible to operate the reactor at high GHSV, at almost complete conversion, achieving process intensification.

2. Materials and Methods

A mathematical model was developed to design the electrically (Joule) heated e-MR reactor for NH_3 decomposition. The model represents a packed-foam reactor integrated with a Pd-Ag membrane through mass, energy, and momentum balances. The kinetics of Franchi et al. (2 wt.% Pt/Al_2O_3) [2] and the membrane parameters of Ongis et al. [3] were implemented. The reactor performance is quantified considering two KPIs: NH_3 conversion and Hydrogen Recovery Factor ($HRF = H_{2,\,perm}/(1.5 \cdot NH_{3,\,in})$).

3. Results and Discussion

Figure 1 reports NH_3 conversion (A) and *HRF* (B) as a function of inlet temperature for an isothermal packed bed (isoT-PB), an isothermal membrane reactor (isoT-MR), and an electrified membrane reactor (e-MR) with different power distributions.

The reactors were simulated under the following operating conditions: $GHSV$=6 $Nm^3/h/kg_{cat}$; p_{ret}=20 bar; p_{perm}=1 bar; membrane surface-to-catalytic bed volume ratio $S_{V,m}$=60 1/m. The isoT-MR reaches the equilibrium conversion of the conventional isoT-PB at a temperature nearly 100 °C lower. Moreover, H_2 removal shifts the thermodynamic limit, allowing the isoT-MR to achieve complete conversion and maximum *HRF* at T_{in}=500 °C. Hydrogen separation through the Pd-Ag membrane allows overcoming the kinetic limitation caused by H_2 occupation of the catalyst active sites.

Regarding the challenge of effectively supplying heat to sustain the endothermic NH_3 decomposition reaction, Joule heating is considered one of the most effective technologies, as it solves the heat-transfer limitations that characterize conventional reactors. Nevertheless, Figure 1 shows that the NH_3 conversion and *HRF* of the electrified reactor (symbols) drop compared to the ideal case of the isoT-MR (solid line). The performance drop of the e-MR can be explained by the mismatch between the variable heat demand along the axial coordinate (proportional to the reaction rate) and the constant volumetric heat supply (q_v) generated by the Joule effect within a single resistive element, as represented in Figure 1C.

By tailoring the resistive element design and/or its power supply, it is possible to obtain a variable (segmented) power input along the reactor axial coordinate, resulting in better coupling of heat demand and supply, and improving both conversion and *HRF*. The combination of H_2 separation and effective heat supply results, for the 4-segment e-MR, in an NH_3 conversion of 95 % and *HRF*=85 % at T_{in}=500 °C, making this reactor configuration approach the ideal case of the isoT-MR reactor.



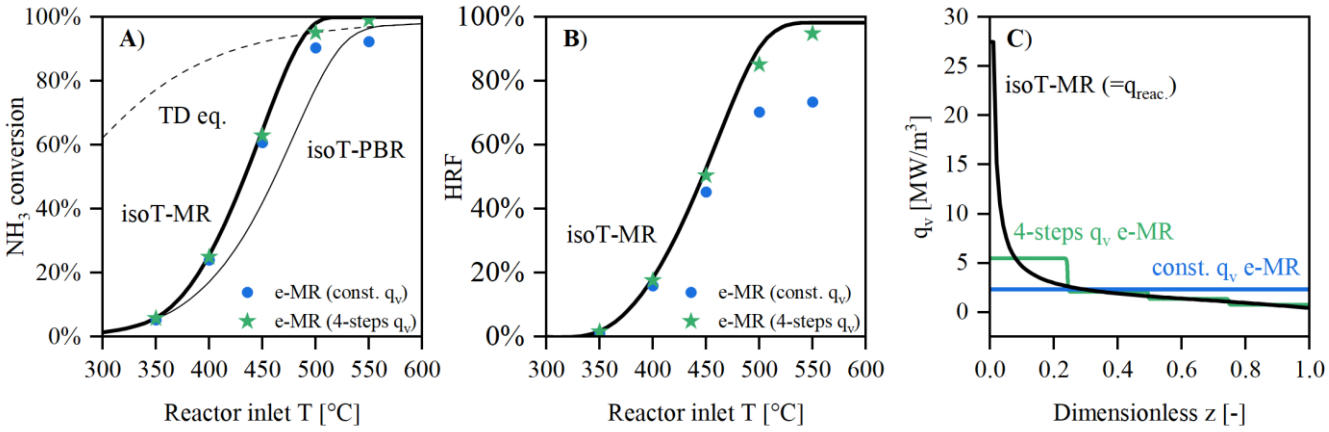


Figure 1: NH_3 conversion (A), *HRF* (B), and q_v distribution at T_{in}=500 °C (C) for different reactor configurations. Simulated conditions: *GHSV*=6 $Nm^3/h/kg_{cat}$; $p_{ret.}$=20 bar; $p_{perm.}$=1 bar; $S_{V,m}$=60 1/m.

4. Conclusions

The proposed electrified membrane reactor effectively couples H_2 separation and tailored Joule heating to overcome kinetic and thermal limitations in NH_3 decomposition. Segmented power input improves heat management, enabling high conversion and *HRF* at 500 °C, approaching ideal isothermal performance and enhancing process intensification. The q_v segmentation proposed in this work is symmetrical along the reactor axis; as a further step, the q_v distribution could be optimized to better match the local heat demand and further improve reactor efficiency.

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CFD STUDY OF AMMONIA SYNTHESIS AND CRACKING IN MEMBRANE REACTOR WITH PERIODIC OPEN CELLULAR STRUCTURE, FOR LONG-TERM HYDROGEN STORAGE - (C073)

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Keywords: Membrane reactors, additive manufacturing, hydrogen, ammonia

1. Introduction

Ammonia is gaining interest for hydrogen storage, thanks to its high volumetric energy content and the ease of its catalytic decomposition [1]. For this purpose, two reactions are involved: ammonia synthesis and cracking. The present work focuses on the combination of two technologies: catalytic membrane reactors that are gaining interest in Power-To-X application [2], and Periodic Open Cellular Structures (POCS) as catalyst support [3]. This study aims to understand external mass transfer in POCS membrane reactors during ammonia synthesis and cracking. Computational Fluid Dynamics (CFD) modeling was supported by laboratory experiments to assess different POCS topologies and evaluating membrane reactor performance.

2. Materials and Methods

CFD simulations were conducted using ANSYS Fluent to study the influence of various parameters on reactor performances. For both synthesis and cracking, reaction rate was derived from literature expression and fitted with experimental data. For this purpose, a POCS sample was tested experimentally as catalyst support, and the same geometry was simulated with CFD. The CFD model was then applied to study segments of POCS membrane reactors with various structures (Kelvin, Body-Centered-Cubic (BCC), and gyroid).

3. Results and Discussion

For ammonia synthesis, the catalytic performance of the structured catalyst BCC was evaluated across a temperature range of 350-600 °C. The model accurately captures the experimental trend of hydrogen conversion, rising from 350 °C to 450 °C and then declining beyond 450 °C. For ammonia cracking, the catalytic performance was assessed on a Kelvin cell, over a temperature range from 400 to 600 °C, on which the model well depicts the conversion increase.

The synthesis CFD model was used to perform simulations on reactors with various POCS structures and various membrane permeance. On the one hand, three POCS reactors were studied (with Kelvin, BCC and gyroid structures), but keeping the porosity and the specific surface area constant. Results show no significant performance difference for the three structures. On the other hand, a membrane POCS reactor with BCC structure was simulated with various permeances. Increasing the permeance improved conversion and recovery, though not linearly as a plateau-like trend was observed, likely due to insufficient ammonia production relative to its removal and strong concentration polarization.

The cracking CFD model was then used to perform simulations on membrane reactors with various gas flowrates and POCS porosities. On the one hand, results show that total hydrogen production continuously increases with gas velocity, while hydrogen flux recovered through membrane reaches a peak at a Gas Hourly Space Velocity of 1850 h^{-1}. On the other hand, decreasing POCS



porosity has two effects on the hydrogen recovery: it increases the catalyst surface (favorable to reaction), and increases reactor obstruction (unfavorable to membrane recovery). These two effects lead to a peak of hydrogen recovery, at a porosity of 0.8 with the tested conditions.

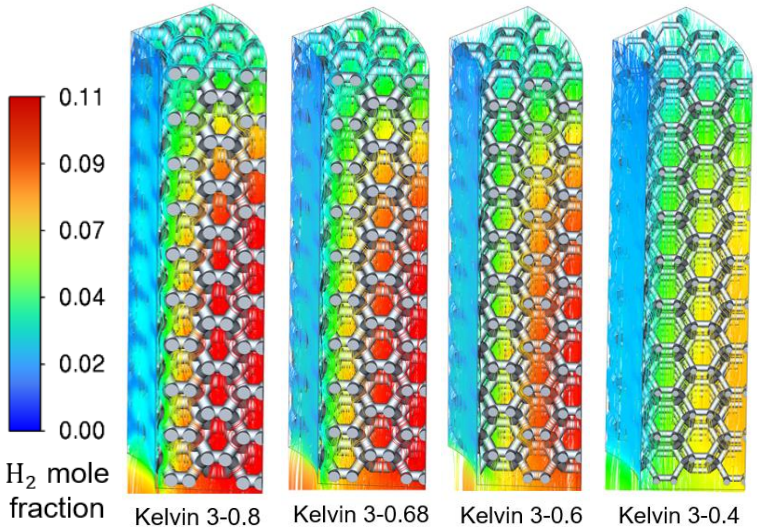


Figure 4 : Streamlines colored with $\mathbf{H_2}$ fraction, on 4 Kelvin structures with various strut diameters (0.8 0.68 0.6 and 0.4 mm)

4. Conclusions

Two numerical CFD models of ammonia synthesis and cracking were validated experimentally and then used to assess membrane POCS reactor performances on ammonia synthesis and cracking. Results show mainly that the type of POCS support does not influence catalytic activity for ammonia synthesis, and that an optimal value of gas velocity and POCS porosity exists to maximize ammonia cracking.

Acknowledgements

Funded by the European Union

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PLATINUM BASED CATHODE FOR HYDROGEN PRODUCTION THROUGH PLASMA-BASED SYNTHESIS - (C074)

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Keywords: Hydrogen, plasma, low loading Platinum, hydrogen evolution reaction, AEM-WE.

1. Introduction

Green hydrogen plays a crucial role in the energy transition, acting both as an energy carrier, derived from non-continuous renewable sources, and as a key reagent for hard-to-abate industries such as steel and fertilizer ones [1]. Among the technologies to produce green H_2, anion exchange membrane water electrolysis (AEM-WE) could exploit abundant material for Hydrogen Evolution Reaction (HER), but Platinum is still largely used, often requiring high loadings ($\geq$0.5 mg/cm^2). State-of-the-art electrodes are typically produced via wet-chemistry routes, involving solvents and multiple steps. This work proposes a plasma-based fabrication route of low-Pt-loading cathodes for HER in AEM-WE, enabling solvent-free, fast and scalable depositions, while maintaining good catalytic activity.

2. Materials and Methods

Electrodes were fabricated starting from carbon cloth (AvCarb – 1071HCB) coated with carbon nano-onions (CNOs) via NanoJeD™ [2]. Pt was deposited by RF magnetron sputtering using a home-built reactor. Morphology and Pt loading were evaluated by SEM and TGA respectively, while catalytic performance by LSV, CV and EIS, carried out in 1 M KOH using a three-electrode setup with Ni foam counter electrode, Hg/HgO reference electrode, and a 0.7 cm² working electrode. iR correction is applied to every measurement.

3. Results and Discussion

Carbon cloth (CC) is a widely used carbonaceous substrate as Gas Diffusion Layer (GDL) thanks to its good electrical conductivity, although it possesses a relatively low surface area. To enhance its this property, a 3 µm thick layer of CNOs is deposited via the NanoJeD™ technique [2]. In this process, a dusty Ar/C_2H_2 plasma is ignited, inducing the formation of polyacetylene nanoparticles that are accelerated toward the substrate through a difference in pressure. Subsequent vacuum annealing converts these particles into CNOs producing a high surface area substrate (CC_CNOs), with a significant morphological modification shown in Fig 1a, 1b. To evaluate the electrochemical surface area (ECSA), Platinum is deposited by RF magnetron sputtering with a nominal thickness of 50 nm (0.1 mg/cm²) and hydrogen underpotential deposition (HUPD) measurement is performed. As reported in Table 1, coated samples exhibit higher ECSA values, which translate into improved catalytic performance, so in a lower overpotential (η) at 10 mA/cm². These results demonstrate that the deposition of CNOs effectively increases surface area enhancing catalytic activity. After confirming the beneficial role of the CNOs layer, the Pt loading effect is studied by varying the sputtering time. As shown in Table 1, despite the higher Pt amount, the 0,4 mg/cm² sample shows worse catalytic activity, with increased η @ 10 mA/cm². This behavior



can be attributed to partial blocking of the porous structure and reduced accessibility of active sites. This is confirmed by observing that for 0.05 mg/cm^2 (Fig. 1c) the original morphology of the CNOs is conserved, while for 0.4 mg/cm^2 (Fig. 1d) the pores are blocked by Pt. The optimal loading is found at 0.3 mg/cm^2, where the best balance between platinum

amount and accessibility of active sites is achieved.

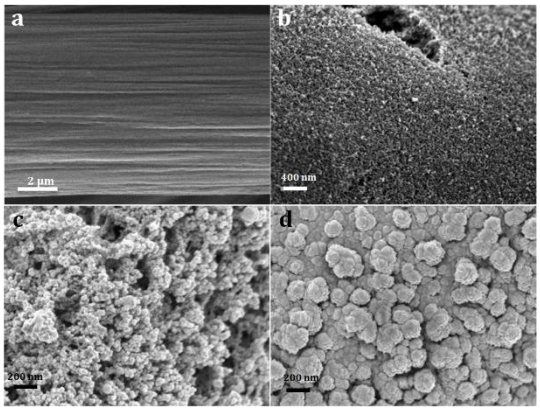


Figure 1. SEM micrograph of the produced sample. a) pristine carbon cloth, b) CNOs layer as deposited, c) CC_CNOs with 0.05 mg/cm^2 of sputtered Pt, d) CC_CNOs with 0.4 mg/cm^2 of sputtered Pt.

substrate	Pt loading [mg/cm^2]	η [mV]	ECSA [cm^2]
CC	0.05	80	4.3
CC_CNOs	0.05	69	12.9
CC_CNOs	0.1	62	14
CC_CNOs	0.2	50	28.5
CC_CNOs	0.3	47	36.1
CC_CNOs	0.4	56	26

Table 1. Loading, η @ 10 mA/cm^2 and ECSA for each sample

4. Conclusions

In this work a fast and reliable production of a working cathode for HER through plasma routes is established. We demonstrated how CNOs can increase the surface area of a commonly used CC, thus decreasing the overpotential of the reaction. Moreover, the Pt loading effect is studied, showing that a balance between Pt amount and accessibility of the active sites is found for 0.3 mg/cm^2. This work must be extended to improve better performances at even lower Pt loadings.

Acknowledgements

This work was supported by X-nano s.r.l. and Flow-nano s.r.l. L.V.D. is funded through a fellowship related to the National recovery and resilience Plan (PNRR), DM 117, Mission 4, Component 2 “From Research to Business” – Investment 3.3 “Introduction of innovative doctorates that meet the innovation needs of businesses and promote the hiring of researchers by businesses”.



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$NiFe_2O_4$ AS AN EFFICIENT AND STABLE ANODE FOR AEM WATER ELECTROLYSERS - (C075)

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Keywords: nickel ferrite catalysts, anionic exchange membrane, electrolyser, oxygen evolution reaction.

1. Introduction

Anion exchange membrane (AEM) water electrolysis is gaining attention as a cost-effective route for green hydrogen production, merging the benefits of alkaline systems with the compact architecture of PEM devices. Its alkaline operation enables the use of earth-abundant OER catalysts, though durability and activity remain limiting factors. Here, we explore $NiFe_2O_4$ as a scalable OER catalyst prepared via a modified oxalate synthesis [1] and evaluated in a single-cell AEM electrolyser.

2. Materials and Methods

$NiFe_2O_4$ was synthesized by sequentially adding nickel and iron nitrates to oxalic acid, followed by H_2O_2-assisted precipitation. After filtration and drying, the precursor was calcined at 350 °C [2]. The catalyst was spray-coated onto a PiperION® (40 µm, Versogen) membrane to form the anode and tested in a 5 cm^2 AEM cell with a Pt cathode. Different loadings were investigated.

3. Results and Discussion

The modified oxalate route yielded phase-pure $NiFe_2O_4$ after low-temperature calcination, providing a homogeneous and finely dispersed oxide suitable for electrode fabrication. Spray deposition enabled uniform catalyst layers directly on the membrane surface, ensuring good interfacial contact within the membrane electrode assembly.

Electrochemical tests in a 5 cm^2 single-cell AEM electrolyser demonstrated that $NiFeO_x$ loading significantly influences performance. The optimized electrode exhibited competitive OER activity compared to literature data for Ni–Fe-based oxides under similar operating conditions.

Preliminary stability tests indicated stable cell operation over extended periods, suggesting adequate structural robustness of the nickel ferrite under alkaline electrolysis conditions. These results confirm that $NiFe_2O_4$, synthesized via a simple and scalable method, can serve as an effective non-precious OER catalyst in AEM electrolysers.

4. Conclusions

$NiFe_2O_4$ prepared by a modified oxalate method demonstrated promising OER activity and stability in a 5 cm^2 AEM electrolyser. The results highlight the potential of nickel ferrite as a cost-effective and scalable alternative to noble-metal-based anodes in AEM water electrolysis.

Acknowledgements

This work was supported by the Italian Ministry of Foreign Affairs and International Cooperation (MAECI) within the framework of the Italian-German joint research initiative "Green Hydrogen Research: A Collaboration to Empower Tomorrow's Energy", under



the project DURALYS (DURAble, Scalable, and Recyclable Components and Cell Designs for Next Generation Alkaline Exchange Membrane Water Electrolysis).

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ENVIRONMENTAL ANALYSIS OF A NANOWIRE LEAD-ACID BATTERY CELL - (C076)

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Keywords: Life Cycle Assessment, Lead-acid batteries, Nanowire, Lab-scale.

1• Introduction

Lead-acid batteries continue to play a key role in stationary storage, due to their high recyclability and operational reliability despite a limited specific energy (35-40 Wh/kg) compared to lithium-ion counterparts (90-300 Wh/kg) [1]. To bridge this gap, nanowire-based electrodes have emerged as a promising solution, increasing the active surface area by up to 70 times and significantly enhancing charge kinetics [2]. However, the environmental implications of these nanostructured components are not yet fully quantified. This study provides a lab-scale Life Cycle Assessment (LCA) to evaluate the environmental burdens of nanowire fabrication, offering a benchmark for the early-stage development of this technology.

2. Materials and Methods

The LCA adopts a cradle-to-gate approach examining the Global Warming Potential (GWP) and the Global Energy Requirement (GER) indicators. The functional unit is defined as one laboratory-scale lead-acid battery cell, encompassing all materials and energy flows required for its assembly. The Life Cycle Inventory is compiled using primary experimental data and secondary data from Ecoinvent database [3].

3. Results and Discussion

The LCA results show a climate change impact of 4.37 kg CO_2 eq, characterized by a distinct distribution of impacts across components. As illustrated in **Errore. L'origine riferimento non è stata trovata.**, the impact is primarily driven by the electrodes, which combined account for 61% of the total (anode: 31%; cathode: 30%). This significant contribution is directly linked to the synthesis of nanowire electrodes, where chemical precursors represent the major hotspots. The battery case contributes a comparable share (30%), indicating that at the laboratory scale, structural materials can be as impactful as the electrochemical components. The total primary energy demand (GER) is 78.89 MJ. Here, a different trend emerges: the battery case represents the dominant hotspot (48%), while the anode and cathode show a lower combined share (41%). This discrepancy is attributed mainly to the typical mass imbalance of lab-scale prototypes, where the housing often outweighs the small quantities of active nanomaterials. The contribution of lead, electrolyte, packaging, and separators remains marginal (below 10% total) for both GER and GWP.



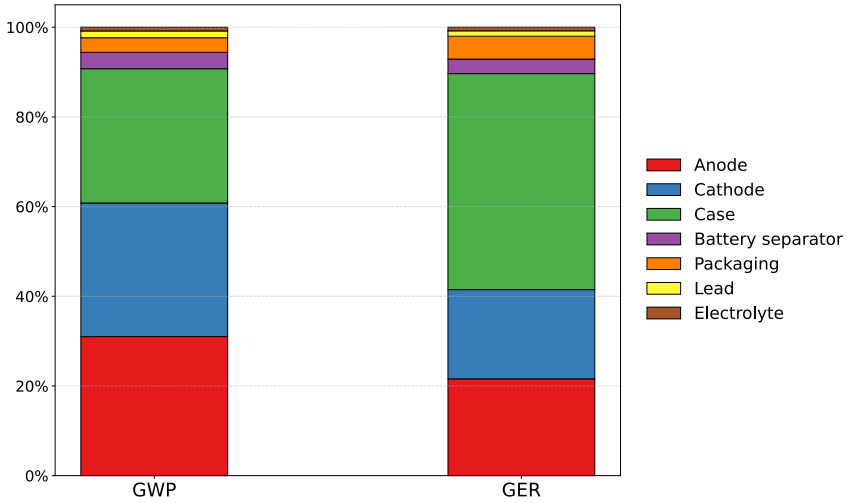


Figure 5 Contribution analysis of the battery cell

4. Conclusions

This study assessed the environmental impacts of the nanowire lead-acid battery cell, focusing on GER and GWP indicators. By identifying electrode fabrication and structural components as the hotspots, these findings enrich the current lack of LCA data for nanostructured battery components. Despite the limitations of lab-scale data, this work offers a preparatory framework to support future scale-up processes.

Acknowledgements

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ROBUST Fe/C CATALYSTS FROM SIMPLE PREPARATION FOR STABLE AMMONIA DECOMPOSITION - (C078)

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Keywords: Ammonia, decomposition, hydrogen, iron, carbon

1. Introduction

Ammonia is a promising hydrogen carrier thanks to its high volumetric H_2 density, existing infrastructure, and carbon-free. On-site cracking can deliver CO_x-free H_2 for fuel cells and industry but requires inexpensive catalysts that reach high conversion at moderate temperature and remain stable. Fe-based systems are attractive for cost, yet their performance strongly depends on the support[1]. Carbon supports tune metal dispersion, but many are unstable under harsh NH_3/H_2 environments, so crystalline carbons are often used[2]. Here we report an active, durable Fe catalyst on non-crystalline carbon. By screening carbon precursors and Fe loadings, we identify an optimized formulation that can serve as a platform for future N-stabilized designs.

2. Materials and Methods

Melamine and dicyandiamide were treated at 550 °C for 3 h to obtain carbon supports followed by Fe deposition by wet impregnation. ICP-OES analyses were performed using an iCAP PRO instrument, Raman spectra were collected with a Confocal DXR3 microscope, and HRTEM pics were taken with a JEM-F200. An Altamira microBenchCat automated test unit was used to evaluate the activity with pure NH_3 between 250°C and 600°C at a space velocity (SV) of 15k mL/g ∗ h. Stability was evaluated at 500 °C by varying the SV between 12k and 6k mL/g ∗ h.

3. Results and Discussion

Fe-based catalysts were synthesized from melamine (Fe-m), dicyandiamide (Fe-d), and their combination (Fe-dm) at different metal loadings. All samples were active in NH_3 decomposition, achieving at 500 °C and SV of 15k mL/g ∗ h conversions comparable to those reported for analogous systems based on crystalline or ordered carbon supports (between 50-70%) (Figure 1a). Among them, Fe-dm was the most performant, reaching 68% conversion and exhibiting a TOF ~70% higher than the other formulations. Crucially, Fe-dm also showed the highest stability at 500 °C during 20 h time-on-stream tests, including under step changes in space velocity. These differences originate from the distinct evolution of the support during the H_2 pretreatment at 600 °C prior to NH_3 feeding. As shown in Figure 1d,e, the as-prepared Fe-dm consists of Fe nanoparticles dispersed on lamellar C/N structures, which undergo substantial restructuring upon reduction, consistent with Raman analysis (Figure 1f) and XRD (not shown). The fresh catalyst displayed bands at ~1600 and ~1230 cm^{-1}, assigned to C–N stretching and skeletal vibrations of carbon nitride; after H_2 treatment these features vanish and a dominant D band at ~1317 cm^{-1} emerges, indicating predominantly disordered sp^2 carbon. In parallel, low-frequency bands associated with Fe-containing phases become more pronounced, in agreement with HRTEM evidence of highly dispersed Fe nanodomains. Notably, only Fe-dm retains a carbonaceous matrix after H_2 treatment, whereas in the other



catalysts carbon is largely lost. The preserved carbon likely contributes to improved dispersion and stabilization of Fe nanoparticles, explaining the superior activity and durability of Fe-dm.

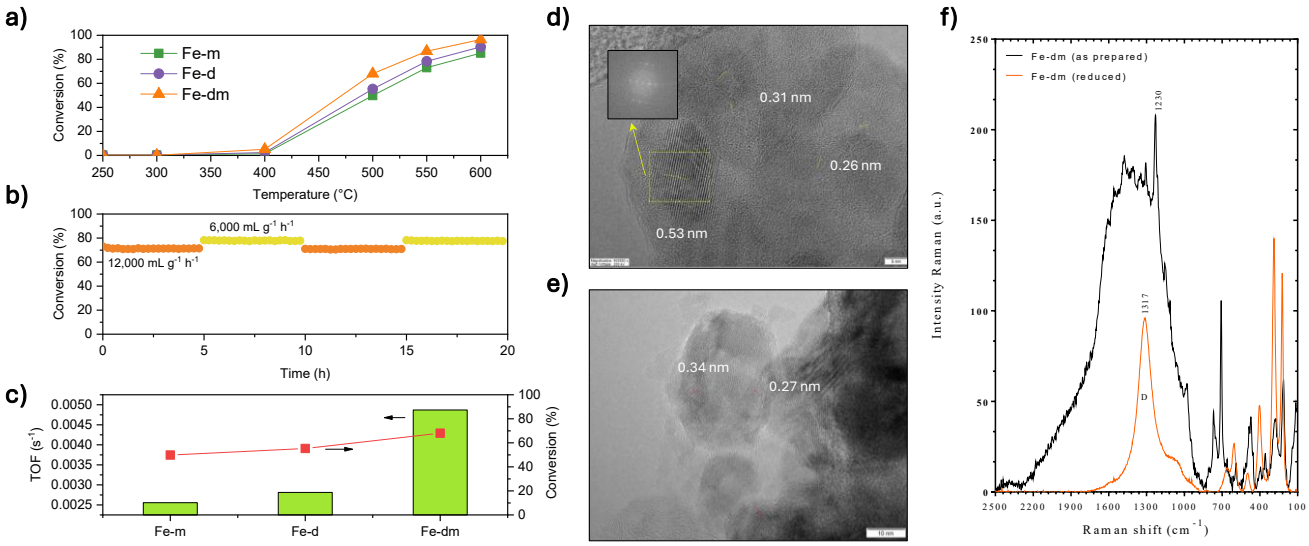


*Figure 1. Conversion up to 600 °C at SV of 15k mL/g * h (a); stability tests at 500 °C and SV of 12k and 6k mL/g * h (b); HRTEM images (d and e) and Raman spectra (f) of Fe-dm as prepared and reduced, respectively.*

4. Conclusions

In this work we developed an active and stable Fe catalysts on non-crystalline carbon for pure NH_3 decomposition. Fe-dm formulation performed best (68% conversion at 500 °C; TOF ~70% higher) and was stable for 20 h despite space-velocity changes. H_2 pretreatment converts its lamellar C/N matrix into retained disordered carbon, dispersing Fe nanodomains. Further gains, especially at lower reaction temperatures, will require stabilizing N sites.

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KINETIC AND MECHANISTIC STUDY OF NH_3 DECOMPOSITION OVER HIGHLY ACTIVE Ru/CeO_2 CATALYSTS - (C079)

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Keywords: NH_3 decomposition, kinetics, ceria catalysts.

1. Introduction

Green NH_3 will play a major role in the future energy transition as H_2 carrier[1]. Ru is widely recognized as the most active metal phase for NH_3 decomposition, but the choice of support also plays a major role[2]. CeO_2 is emerging as promising support for NH_3 cracking thanks to its ability to provide strong metal-support interactions (MSI) and increased electron mobility[3]. This work aims to evaluate the performances of Ru/CeO_2 catalyst both with diluted and concentrated NH_3 feed and develop robust and fundamental-based kinetic models. A reference $Ru/\gamma Al_2O_3$ formulation was adopted for comparison.

2. Materials and Methods

$1\%Ru/CeO_2$ and $1\%Ru/Al_2O_3$ catalysts were prepared by IWI, using $Ru(NO)(NO_3)_3$. Catalysts were characterized by BET, H_2 TPR, CO chemisorption and XRD. NH_3 cracking was carried out in micro-fixed bed unit under diluted and concentrated NH_3 feed up to $50\%NH_3$/He at GHSV 20000-80000 $Nl/h/kg_{cat}$. Product co-feeding tests were performed. DRIFTS experiments were performed to elucidate reaction intermediates and H* interaction with the support. Kinetic modelling was based on 1D pseudo-homogeneous reactor model.

3. Results and Discussion

Characterization shows high dispersion for both Ru/CeO_2 and Ru/Al_2O_3 catalysts. Activity results in the $1\%NH_3$ and $1\%NH_3$+$25\%H_2$ conditions at 20000 Nl/h/kgcat are shown in Errore. L'origine riferimento non è stata trovata.**a**. Ceria-based catalysts outperformed Ru/Al_2O_3 catalysts: at 300°C conversion increased from 15% to 80% in the $1\%NH_3$ condition.

Reduced hydrogen inhibition is preliminary observed from activity data: at about 60% conversion, the temperature shift from 1% NH_3 to 1% NH_3 + 25% H_2 is 95 °C for Ru/CeO_2, compared to 114 °C for Ru/Al_2O_2. The observation was confirmed by H_2 TPD experiments and H_2/D_2 isotopic experiments followed by in situ DRIFTS, which confirmed increased hydrogen storage capacity and mobility of CeO_2.This support promotes H* transfer from the metal to the support, alleviating hydrogen poisoning and increasing reaction rates.

The pseudo-first order analysis of the $1\%NH_3$ experiments reported in Errore. L'origine riferimento non è stata trovata.**b** revealed a two-slope trend for Ru/CeO_2 catalyst, associated with a change in kinetics with temperature. Ru/Al_2O_3 data were described assuming NH_3 activation as Rate-Determining-Step (RDS) with H* adsorbed on the catalyst surface throughout the operative temperature range, while for Ru/CeO_2 a change in the RDS from N_2desorption to NH_3 activation from low to high temperature respectively. The kinetic assumptions were supported by NH_3-TPD experiments aimed at estimating the nature and amount of adsorbed surface species, as well as by in situ DRIFTS measurements performed during NH_3 decomposition at different temperatures to identify reaction intermediates. An overall kinetic model incorporating the two kinetic regimes was developed, and the kinetic parameters were estimated from experiments conducted under diluted, isothermal conditions. The model was subsequently used to predict NH_3 conversion curves at higher concentrations, which were then validated experimentally.



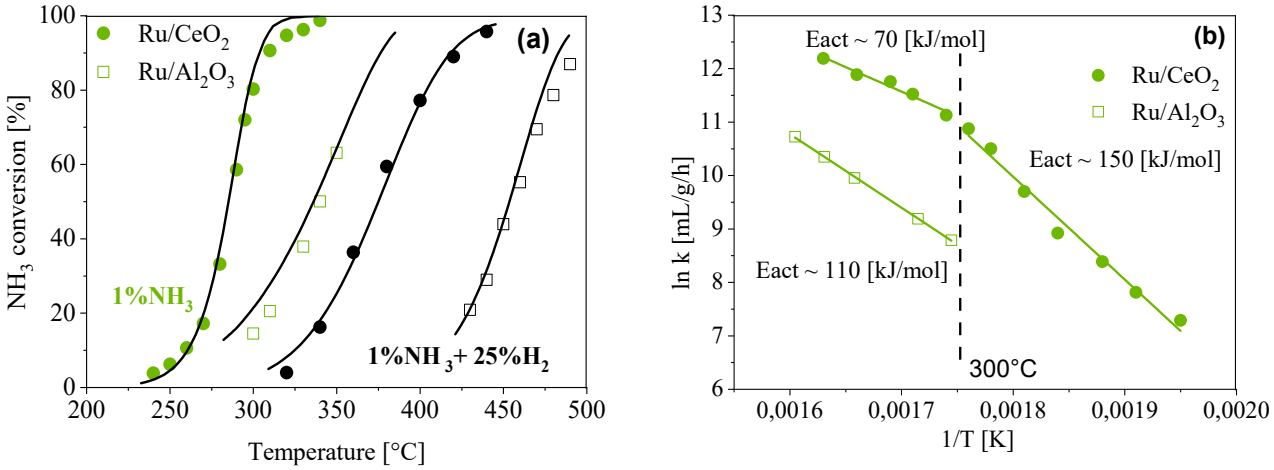


Figure 6 (a) Activity and modelling results for Ru/CeO_2 and Ru/Al_2O_3 catalysts ($1\%NH_3$ and $1\%NH_3 + 25\%H_2$ feed - 20000 $Nl/h/Kg_{cat}$) (b) Pseudo-first order analysis of 1% NH_3 data - 20000 $Nl/h/Kg_{cat}$

4. Conclusions

Ru/CeO_2 catalysts showed enhanced catalytic activity for NH_3 decomposition, associated with the ability of Ru to displace H* from the metal to the support, therefore alleviating hydrogen poisoning. The kinetic analysis revealed a change in the kinetics with temperature for Ru/CeO_2 catalyst, from N_2 desorption at low temperature to NH_3 activation at high temperature. A robust kinetic model was derived from diluted data and validated in more representative conditions up to 50% NH_3/Ar.

Acknowledgements

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INVESTIGATION OF STEAM-IRON PROCESS FOR HYDROGEN STORAGE OVER FUSED Fe-BASED MATERIALS - (C080)

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Keywords: Steam-iron process, Hydrogen storage, Red-Ox cycles.

1. Introduction

Hydrogen is attracting growing interest as an efficient and clean energy carrier. To overcome H_2 storage challenges, the steam–iron process has emerged as a promising solution. Here H_2 is indirectly stored and released through cyclic reactions of charging where Fe_3O_4 is reduced to metallic Fe ($Fe_3O_4+4H_2 \rightarrow 3Fe+4H_2O$), and discharging where Fe is oxidized by water vapor, generating H_2 ($3Fe+4H_2O \rightarrow Fe_3O_4+4H_2$), as shown in Fig.1a [1,2]. This work investigates the steam–iron process over Fe-based materials prepared by fusion–decomposition [3].

2. Materials and Methods

Fe-based materials with varying Fe loading were prepared by fusion-decomposition of the nitrate precursors. Reduced and oxidized samples were characterized by BET, SEM, XRF, XRD. Redox experiments were carried out in TGA and packed-bed reactor.

3. Results and Discussion

The textural characterization of the fused materials (Fig. 1b) indicates appreciably high surface area (30-50 m^2/g), mesoporosity and small Fe-crystallites (< 30 nm), suggesting an adequate Fe dispersion.

a **b**

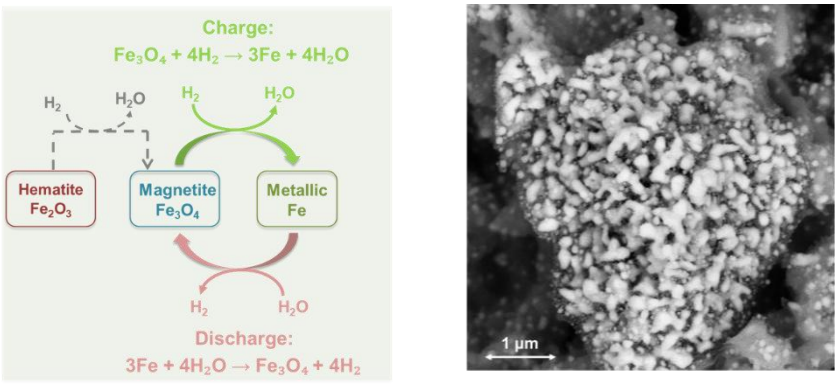


Figure 1. a) Scheme of steam-iron process; b) SEM image of the reduced Fe-based materials.



Isothermal and T-ramping reductions in TGA (Fig. 2a) reveal the positive effect of temperature on the Degree of Reduction (DOR), but also its time-dependence. Indeed, the kinetics of reduction are complex and their comprehension is crucial for the efficiency of the entire process. Based on our results, they positively depend on Fe dispersion and H_2 partial pressure, but negatively on H_2O content. Besides, it was observed that lower reduction temperature leads to faster subsequent oxidation (Fig. 2b). This suggests that the reduction conditions affect the oxidation kinetics by modulating the Fe accessibility. Ongoing research aims at identifying optimal temperature and gas-phase conditions for reduction and oxidation, as well as developing comprehensive kinetics to address reactor design.

a **b**

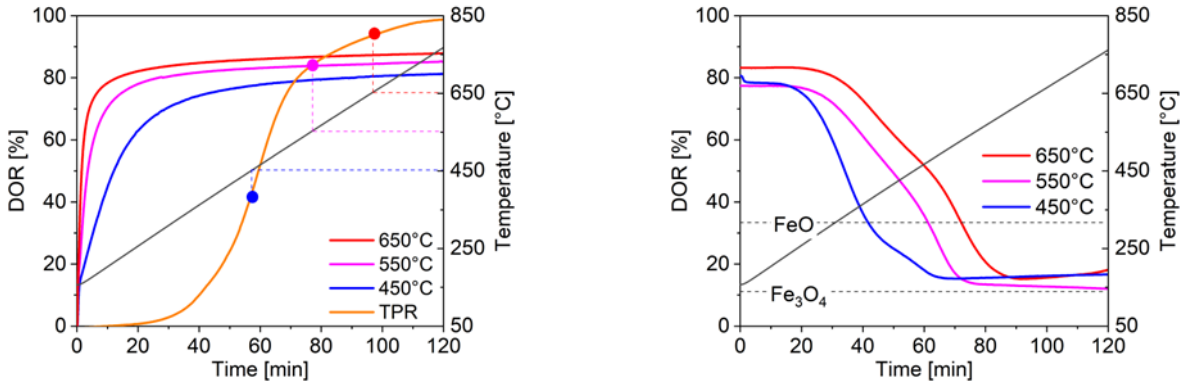


Figure 2. a) Effect of temperature on reduction of Fe_2O_3 to Fe; b) Effect of reduction temperature on temperature-programmed oxidation from reduced sample to Fe_3O4. Temperature program: 150-800°C, 5°C/min; total flow rate: 150 Nml/min.

4. Conclusions

The reduction and oxidation steps of steam-iron process were investigated on Fe-based materials prepared by fusion-decomposition. Both temperature and gas-phase composition affect reduction and oxidation kinetics, opening further research to identify optimal conditions for reactor design. Cycling tests are on-going to assess the performance of these materials over longer duration.

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ELECTRIFIED REVERSE WATER GAS SHIFT: AN EXPERIMENTAL AND MODELLING STUDY ON A JOULE-HEATED PACKED FOAM REACTOR. - (C082)

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Keywords: Electrified reactors; Reverse Water Gas Shift; Joule-heating; CO_2 valorization.

1. Introduction

In a world committed to reducing CO_2 emissions, the production of green syngas via Reverse Water Gas Shift (RWGS) is expected to play an important role to enable the production of "green syngas" that can be further exploited for production of chemicals and fuels. Given the endothermic nature of the RWGS reaction, an electrified reactor that uses renewable electricity to provide high-temperature heat allows to completely eliminate CO_2 emissions from combustion processes. In this work we provide an in-depth experimental and modelling analysis of a directly Joule-heated Silicon infiltrated Silicon Carbide (SiSiC) foam packed with Rh catalysts for syngas production, shedding light, for the first time, on the thermal effects of competitive methanation.

2. Materials and Methods

Experimental activities were conducted using a lab-scale reactor where a SiSiC open cell foam (L=100 mm, d = 35mm) was packed with 56 g of Rh-Al_2O_3 catalyst pellets (dp=1mm) by Heraeus. As illustrated in Figure 1a, the SiSiC structure (Engicer SA) was connected to an AC power supply acting as a heating element generating heat in intimate contact with the catalyst [1]. The foam was machined to specifically host some thermocouples to record the axial temperature profiles. Experiments conducted in the lab-scale rig were used to validate a 2D mathematical model of the packed foam reactor that was applied to data analysis and scale up.

3. Results and Discussion

Experimental data demonstrated that our reactor was able to achieve equilibrium CO_2 conversion and CO-selectivity for outlet temperatures in the span [600 – 750 °C], pressures up to 5 bar and space velocities between 6 and 18 $Nm^3//kg_{cat}/h$. In particular, pressures above atmospheric and temperatures below 700°C led to a higher amount of methane in the product stream in line with the predictions of thermodynamic. while ensuring thermal efficiencies up to 76%. Measured axial temperature profiles (Figure 1b) showed the effect of methanation on the temperature distribution at the inlet of the catalytic bed; indeed an increase of 300 °C occurred in the first section of the reactor, for the combined action of Joule-heating and methanation exothermicity, enhanced at higher pressure. Parallelly, kinetic experiments were independently conducted in a temperature-controlled reactor to obtain a kinetic scheme. These data were used to perform a mathematical model of the unit, that closely matches the experimentally recorded temperature profiles. The model will be further employed to design industrial scale units of this reactor concept.



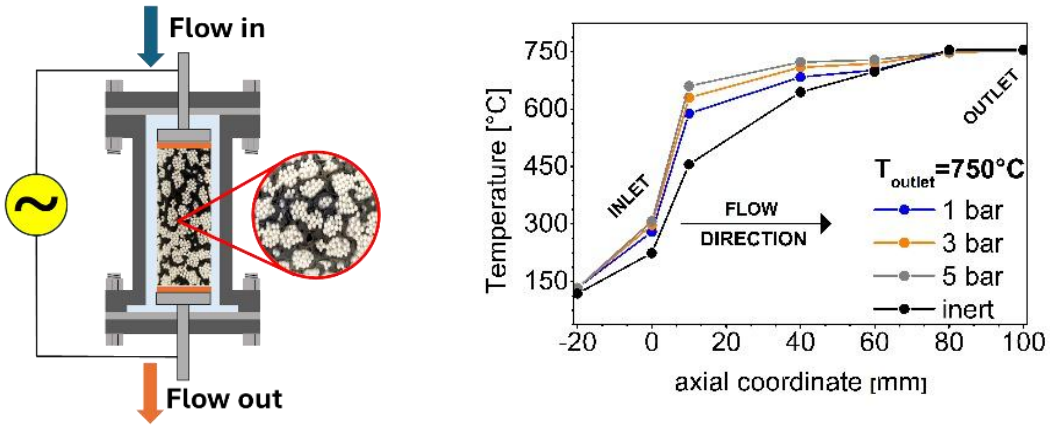


Figure 7 a) scheme of the electrified packed foam reactor and b) effect of operating pressure on the temperature profiles.

4. Conclusions

With this work we propose an application of our concept of electrified reactor which aims at valorizing captured CO_2 by converting it into syngas. Thanks to the presence of a resistive structured catalyst, thermal power can be generated directly in the catalytic bed, allowing to achieve equilibrium conversion up to 18 $Nm^3/kg_{cat}/h$. Temperature profiles allowed to assess the effect that methanation has on the thermal behavior of the reactor which was faithfully described by the mathematical model.

Acknowledgements

Rosetti Marino S.p.A. is acknowledged for funding this project and bringing in scientific contribution.

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ENERGY AND ENVIRONMENTAL PERFORMANCE ASSESSMENT OF A BIO-BASED ELECTRODE MANUFACTURING FOR VANADIUM REDOX FLOW BATTERY - (C083)

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Keywords: LCA, Energy and Environmental Impacts, Bio-based electrode manufacturing, vanadium redox flow battery.

1. Introduction

Electrochemical storage plays a strategic role in enhancing an energy system characterized by high penetration of non-programmable renewable sources, increasing electrification of end-use consumption, and a need for greater grid flexibility, representing one of the pillars of the energy transition. Accordingly, reducing the environmental impact of these technologies is therefore a key element of their sustainability. This requires innovative solutions that, in accordance with European Regulation 2023/1542 on batteries [1], introduce the principles of the circular economy into the system's value chains [2].

2. Materials and Methods

The following research work, in accordance with the ISO 14040 series standards [3], performs a cradle-to-gate Life Cycle Assessment to investigate the energy and environmental performance of a vanadium redox flow battery bio-based electrode, from the extraction of raw materials to the complete production of the electrode. In detail, the electrodes investigated are made from two different waste biomasses: algae and wood chips.

3. Results and Discussion

For both types of electrodes, which share the same production process, the overall gross energy impact varies between 4.4 and 4.5 MJ, and approximately 82% of the total is mainly composed of fossil energy. Regarding the environmental analysis, it emerges that the environmental impact of algae-based electrode is higher than that of woodchip-based electrode in all investigated impact categories, with a variation ranging from 1% (photochemical ozone formation) to 4% (ozone depletion). For example, focusing on climate change impact category, it was estimated a value of 1.68E-01 kg CO_2eq for the algae-based electrode and 1.64E-01 kg CO_2eq for the woodchip-based one, with a difference of 2%. To identify the phases and the "hotspot" elements that contribute most to the impact generation, a dominance analysis was conducted. In detail, the dominance analysis evaluated on the overall gross energy impact shows that the pre-treatment phase approximately has an impact of 19%, pyrolysis of 16%, post-treatment phase of 7% and finally electrode preparation of 59%, identifying it as the phase with the greatest impact of the entire production process. Similarly, from an environmental perspective, although it is not possible to identify a uniquely dominant phase for each impact category, it is possible to state that on average, for both electrodes, the dominant phase is represented by the final electrode preparation phase, with the exception of the human toxicity cancer effects, ionizing radiation, land use, and non-fossil abiotic resources depletion impact categories. Conversely, the least impactful phase in each examined category is the post-treatment phase (Figure 1). Furthermore, detailed analysis of each phase allowed to identify electricity consumption as the main hotspot for all energy and environmental impact categories. The only exception is the final phase of the process, where the dominant impact is generated by isopropanol.



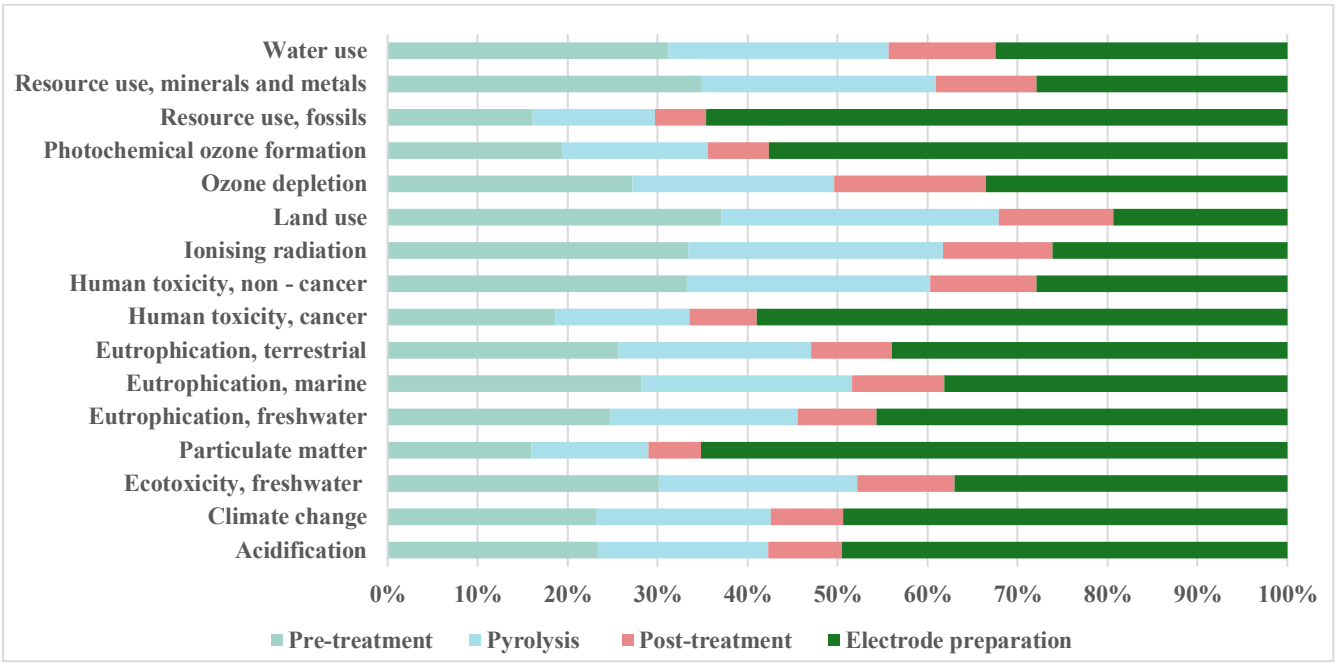


Figure 1. Electrode impact dominance analysis.

4. Conclusions

Ultimately, the obtained outcomes have contributed to enriching the poor literature on Life Cycle Assessment studies applied on vanadium redox flow battery bio-based electrode by identifying the energy and environmental hotspots of the manufacturing process on which to concentrate the greatest efforts of future research.

Acknowledgements

The study was funded within the Integrated Project 1.2 “Electrochemical and thermal storage technologies”, Program Agreement CNR-MASE, RdS PT 2022-2024.

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SCALABLE ELECTROSPINNING SYNTHESIS OF CUO AND Fe_2O_3 ELECTRODES FOR PHOTOELECTROLYSIS - (C084)

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Keywords: Electrospinning, Photocatalysis, PEC cells, Electrolysis.

1. Introduction

Efficient and stable water splitting via photoelectrochemical (PEC) cells requires the development of advanced electrodic materials. Current limitations include low efficiency and durability of hematite (α-Fe_2O_3) photoanodes and CuO photocathodes, often hindered by poor charge transport and stability in aqueous environments [1]. This work addresses these challenges by utilizing electrospinning to synthesize α-Fe_2O_3 and CuO electrodes with optimized geometries and also study the effects of Transition Metal doping on the performances of the photoelectrodes.

2. Materials and Methods

α-Fe_2O_3 photoanodes were fabricated via electrospinning of a PVP solution containing Iron Nitrate as a precursor. Successive thermal treatment was done to ensure the complete carbonization of the polymeric matrix and the formation of hematite fibers on the surface of the FTO glass. Doping of the active phase was done by adding suitable Ti and Sn precursors in the polymeric solutions. Similarly, CuO photocathodes, doped with Fe and Cr, were synthesized starting from a PVA solution and subsequent combustion. The synthesis was done in such a way to obtain a 4 cm^2 electrode surface.

3. Results and Discussion

XRD analysis was done to confirm the formation of the correct phase of oxides on the surfaces of the electrodes, SEM imaging was used to study the morphology of the deposited fibers.

α-Fe_2O_3 photoanodes achieved photocurrents exceeding 1.8 mA/cm^2 under AM 1.5G illumination, CuO photocathodes, doped with Fe and Cr, exhibited photocurrents exceeding 0.9 mA/cm^2 under the same conditions.

4. Conclusions

Electrospinning allowed for the synthesis of electrodes with a peculiar fibrous structure. The addition of doping agents in the structure was also facilitated thanks to the addition of precursors directly in electrospun solution leading to uniform distribution in the final fiber. Electrochemical performances were competitive with other photoelectrodes found in literature. One of the great advantages of this synthesis process lies in the ease of

scalability for the area of the electrodes, that could lead in the near future to a scale up to 10cm^2 and tests inside a complete photoelectrolysis cell.



Acknowledgements

The authors gratefully acknowledge the University of Messina, in particular the XL Cycle of the Ph.D. Program in Engineering, for its institutional and scientific support.

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EMERALD: MODELING AND EXPERIMENTAL VALIDATION OF A NOVEL RADIAL-CURRENT EREACTOR FOR INTENSIFIED ENDOTHERMIC CATALYTIC PROCESSES - (C086)

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Keywords: Electrification, Process Intensification, Innovative Reactor Design

1. Introduction

Electrification of Steam Methane Reforming (eSMR) represents a promising pathway for the decarbonization of hydrogen production. A major challenge in SMR is matching heat supply with the strongly varying heat demand of the reaction, to improve reactor performance and mitigate cold-spot formation. In this work, we propose a novel Joule-heated eSMR reactor based on radial electric current and centrifugal gas flow in an annular packed foam (EMERALD configuration) [1]. The aim is to achieve spatially tailored heat generation that better matches the reaction heat demand, enhancing thermal management and overall reactor efficiency.

2. Materials and Methods

To assess the benefits of the proposed design, comparative simulations were performed for packed-foam reactors with axial and radial configurations using a hybrid heterogeneous hierarchical modeling approach [2]. Detailed 3D CFD simulations were used to derive correlations and parameters for reduced 1D and 2D porous-media models [3]. To validate the reactor concept, a lab-scale EMERALD reactor (catalytic bed volume = 100 mL) was constructed. Temperature profiles were measured using seven thermocouples, while product composition was analyzed with an online MicroGC. The reactor casing's temperature was controlled via an external heating tape.

3. Results and Discussion

Figure 1 compares simulation results for the axial (A) and EMERALD radial (B) configurations under identical operating conditions, assuming adiabatic behavior. The axial configuration exhibits a pronounced cold spot at the reactor inlet (Figure 1A). In contrast, the EMERALD configuration substantially suppresses cold-spot formation (Figure 1B). This is achieved through a spatial power distribution that is highest at the catalytic-bed entrance and decreases with $1/r^2$ (assuming constant electrical resistivity), closely matching the reaction heat demand. Additionally, the radial configuration significantly reduces pressure drop.

Experimentally measured temperature profiles (Figure 2A) were found to be strongly influenced by the net heat flux (Electric power supply – Heat of reaction, Figure 2B). When the net heat flux was negative (external heating dominant), temperatures increased monotonically along the reactor (Profiles 1–6). Under near-adiabatic conditions, flatter temperature profiles were observed (Profiles 7–10). When the net heat flux became positive, local temperature maxima developed inside the bed (Profiles 11–13). For all operating conditions, the measured outlet compositions were close to thermodynamic equilibrium, with methane conversion increasing from 44.6% (Profile 1) to 70.8% (Profile 13). Simplified 1D pseudo-homogeneous and detailed CFD models consistently reproduced the experimental trends, supporting validation of the EMERALD reactor concept.



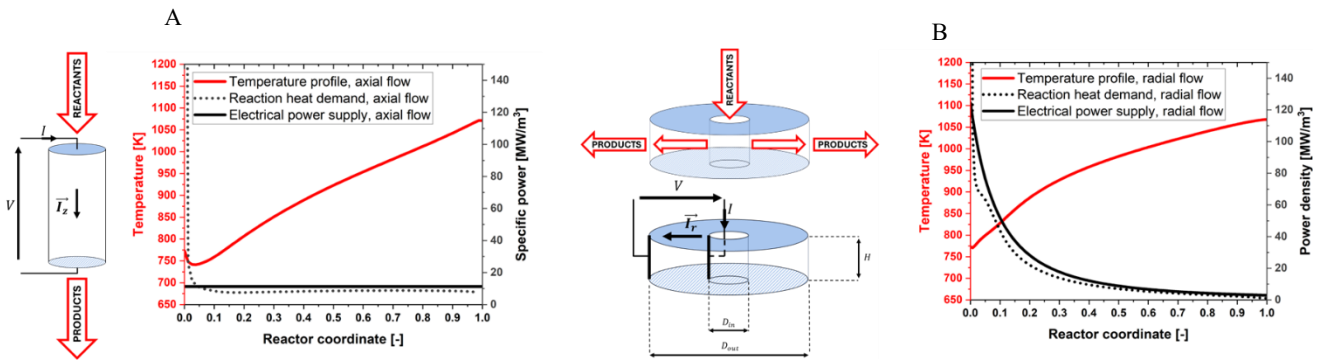


Figure 1. Comparative simulation results: A) Axial configuration B) EMERALD (radial) configuration [1]

(Rh catalyst, GHSV = 20 Nl/h/g_{cat}, H_2O:CH_4:H_2 = 2.5:1:0, V = 21.4 l, Power = 234 kW, T_{in} = 773 K, P = 7 bar)

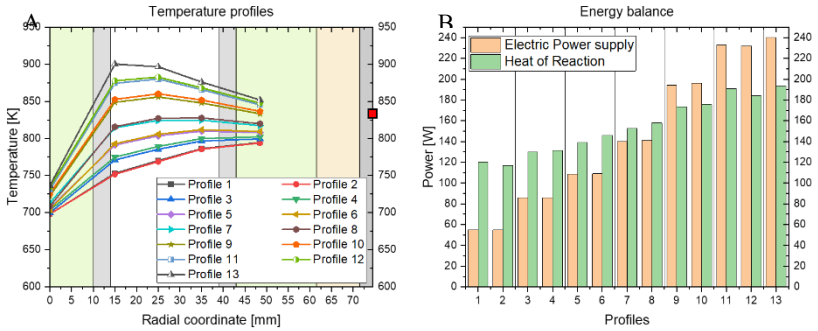


Figure 2. Experimental results: A) Temperature profiles B) Energy balance

(Rh catalyst, GHSV = 5 Nl/h/g_{cat}, H_2O:CH_4 = 3:1, V = 0.1 l, P = 1 bar)

4. Conclusions

The EMERALD Joule-heated radial reactor enables spatially tailored heat generation that matches SMR heat demand, significantly reducing cold-spot formation and pressure drop compared with axial designs. Experimental and modeling results validate the concept and demonstrate its potential for intensified, electrified hydrogen production. Scale-up and optimization studies are in progress.

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The authors acknowledge Air Liquide for their support of this research.

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FLUORINE-FREE POLYMER ELECTROLYTE MEMBRANE FOR ADVANCED HIGH-ELECTROCHEMICAL PERFORMANCES 2 V SOLID-STATE ASYMMETRIC SUPERCAPACITOR - (C087)

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Keywords: Aquivion membrane, Sulfonated polysulfone, Fluorine-free electrolyte membrane, Supercapacitors

1. Introduction

This study describes the successful development and detailed analysis of a series of supercapacitors in asymmetric configurations. The negative and positive electrodes of the asymmetric supercapacitors were fabricated using activated carbon gel and manganese oxide, respectively. All devices were produced in a solid-state configuration using perfluorinated sulfonic acid (PFSA) membranes based on the Aquivion membrane and fluorine-free sulfonated polysulfone membranes that are known as hydrocarbon PEMs. These membranes serve both as the electrolyte and as the electrode separator [1, 2]. Each polymer electrolyte was investigated through physical-chemical characterisation using TGA, DSC, ATR-FTIR and Raman spectroscopy, and thereafter studied in a supercapacitor cell configuration with different operating voltage windows ranging from 1 to 2 V. Although the optimal range was found to be 0–2 V, this is well beyond the 1.23 V required for water decomposition in an neutral aqueous environment. This is made possible, however, by the near-neutral pH of the polymer electrolyte membranes and the equal overpotential of the carbon negative and MnO_2 positive electrodes. As demonstrated in the study, these electrodes work individually in an overvoltage of around 1 V vs NHE, rendering the 0–2 V voltage window effective.

2. Materials and Methods

A commercial Aquivion® E87-05S membrane with a thickness of 50 µm was purchased from Merck – Italy. The sulfonated polysulfone (sPSf) polymer was synthesized according to a procedure based on a mild sulfonation process carried out at 50 °C, followed by the recovery of the polymer by precipitation in a non-solvent ethanol bath. To ensure consistent high ion conductivity and improved electrochemical stability, pristine and composite sPSf membranes, as well as commercial Aquivion membranes, were exchanged in a 1 M aqueous solution of sodium sulfate (Na_2SO_4), converting the sulfonic acid groups to the sodium form ($–SO_3^-Na^+$). This sodium form of the electrolyte membrane is essential for supercapacitor applications in aqueous environments as it allows operation at higher cell voltage windows (up to ~2 V at near-neutral pH), whereas proton-form membranes have lower stable voltage windows of around 1 V. Supercapacitors with different polymer electrolyte membranes were characterized using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS).

3. Results and Discussion

Designed supercapacitors based on different polymer electrolyte membranes, namely Aquivion® E87-05S, sulfonated polysulfone (sPSf) and sulfonated polysulfone composite (sPSf-SiO_2-sulf), were characterised using FTIR, Raman, TGA and DSC, as well as comprehensive electrochemical analyses such as cyclic voltammetry (CV), galvanostatic charge and discharge (GCD) tests, electrochemical impedance spectroscopy (EIS) and self-discharge rate measurements.



The Raman and FTIR spectra of the membranes exhibit characteristic vibrational features, including sulfonated groups, which confirm the successful sulfonation process and are fully consistent with the literature. Furthermore, TGA analyses revealed distinct thermal behaviours: the Aquivion® membrane degrades sharply between 320 and 450 °C, while the sPSf and sPSf–SiO_2-sulf membranes display a multi-step thermal effect with the main step occurring between 350 and 500 °C, corresponding to desulfonation and backbone decomposition.

The electrochemical characterizations by cyclic voltammetry indicates that these solid-state supercapacitors with Aquivion® and sPSf membranes exhibit nearly rectangular profiles even at high cell voltages ranging from 0 to 2 V and maintain their stable voltammograms even more 20,000 cycles under the severe 0-2 V voltage window test as illustrated in **Fig. 1A.**

Self-discharge rates were investigated by charging each device for 3 hours from 0 at 2 V and monitoring voltage decay over 24 hours. The voltage trend shows an initial rapid decline during the first 10 hours, after which it stabilises and reaches a steady-state decline, displaying very slow self-discharge rates. Optimum voltage retention is achieved with devices based on a pristine sulfonated polysulfone (sPSf) polymer electrolyte membrane, as shown in **Fig. 1B**.

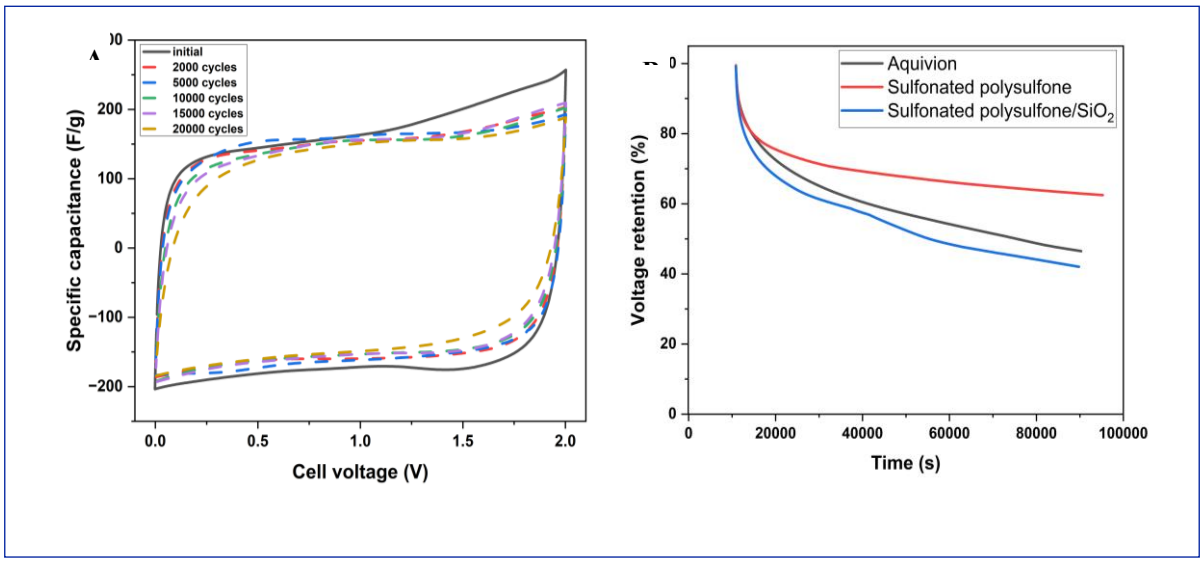


Fig. 1*. CV plot of sulfonated polysulfone membrane during stability test from 0 at 2 V* ***(A)****;* ***(B)*** *self-discharge rates at different cycles for Aquivion, sulfonated polysulfone (SPSf) and composite (SPSf-SiO_2-sulf) membrane.*

4. Conclusions

In this study, carbon xerogels, manganese dioxide (MnO_2) and polymer electrolyte membrane materials were synthesised through a simple, scalable and sustainable approach. Their synergic incorporation of these materials into supercapacitor devices enhanced the devices electrochemical performance, providing excellent cycling stability and reduced self-discharge rates. Devices fabricated with sulfonated polysulfone electrolyte membranes achieved a specific capacitance above 180 $F \cdot g^{-1}$ and an energy density of around 25 $Wh \cdot kg^{-1}$ at a power density of 200 $W \cdot kg^{-1}$, highlighting their potential use in smart devices in the emerging Internet of Things era.

Acknowledgements

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VALORIZATION OF SALTWORKS BITTERN FOR $Mg(OH)_2$ PRODUCTION: A LIFE CYCLE ASSESSMENT - (C091)

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Keywords: Chemicals, LCA, Magnesium hydroxide, Saltworks, By-products

1. Introduction

The valorization of industrial by-products can support the transition toward circular production models. In the salt production sector, large volumes of concentrated bittern are treated as waste despite containing valuable resources as Mg. Life Cycle Assessment (LCA) has been applied to conventional Mg production routes, including thermal decomposition of carbonates and precipitation from saline solutions using chemical reagents [1] [2], highlighting the role of energy demand and process configuration on environmental performance. However, the valorization of bittern remains scarcely explored. The aim of this study is to apply a cradle-to-gate LCA to $Mg(OH)_2$ extraction under reagent-free conditions, addressing the lack of environmental assessments for this recovery pathway.

2. Materials and Methods

The study was conducted in accordance with ISO 14040 and ISO 14044, following the methodological framework of product category rules for basic chemicals [3]. The objective of the study is to evaluate the environmental profile of a process for the recovery of $Mg(OH)_2$ from industrial residual brines. The functional unit was defined as 1 kg of $Mg(OH)_2$ produced at the process outlet. The study focuses on a cradle to gate boundary, including transport of bittern to the processing plant, production and transport of the packaging and the core process, that includes the extraction and production of $Mg(OH)_2$, together with the generation of co-products, hydrochloric acid (HCl) and concentrated brine.

3. Results and Discussion

The preliminary life cycle assessment provides an early understanding of the environmental profile of the proposed $Mg(OH)_2$ recovery pathway. The analysis identifies the main processes that influence the overall impact, highlighting the importance of energy consumption, material input, and waste management within the system boundaries.

The results suggest that the environmental performance of the process is strongly influenced by the configuration of the electricity supply and the material intensity of specific subsystems, particularly packaging. At the same time, the modeling approach adopted for by-products and waste streams plays a significant role in determining the final impact profile.

The assumption applied to brine, considered a by-product of salt production, allows the assessment to focus exclusively on the recovery process itself. This approach provides a consistent basis for evaluating the recovery pathway independently of upstream salt extraction.

The application of allocation procedures highlighted the multifunctional nature of the system, showing that a significant share of environmental burdens is associated with the co-production of HCl. The relatively higher output of HCl compared to $Mg(OH)_2$ leads to a redistribution of impacts across the co-products, resulting in a reduced environmental load attributed to $Mg(OH)_2$. This aspect confirms the relevance of multifunctionality modeling choices in shaping the environmental profile of the recovery pathway and underlines the importance of transparent allocation assumptions in life cycle studies of integrated processes.



4. Conclusions

This study demonstrates the relevance of adopting a life cycle perspective when assessing innovative recovery pathways for industrial by-products. The results confirm that even processes designed under circular and reagent-free configurations may present non-negligible environmental trade-offs, which are strongly influenced by energy supply. The analysis highlights the importance of integrating environmental assessment at early design stages to support eco-design and industrial scale-up.

Acknowledgements

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La(OH)$_3$-IROX CATALYSTS FOR EFFICIENT OXYGEN EVOLUTION REACTION IN ACIDIC ENVIRONMENT - (C092)

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Keywords: iridium, oxygen evolution reaction, lanthanum, water electrolysis.

1. Introduction

Water electrolysis is a key technology for energy decarbonization, enabling the conversion of intermittent renewable electricity into green hydrogen. Proton exchange membrane water electrolyzers (PEMWEs) are attractive due to their high efficiency and hydrogen purity, but the acidic and oxidizing environment requires noble-metal catalysts for the oxygen evolution reaction (OER). Although IrO_2 is the benchmark catalyst, the scarcity and high cost of Ir limit large-scale deployment. Here, IrO_x-La core-shell catalysts synthesized via a simple hydrothermal route are proposed. La incorporation can induce lattice strain and electronic effects that weaken Ir-O bonding, promote oxygen vacancy formation, and stabilize higher Ir oxidation states [1]. These combined effects enhance intrinsic OER activity and improve noble-metal utilization, offering a promising strategy for efficient and durable PEM water electrolysis.

2. Materials and Methods

Ir-La catalysts were synthesized via a two-step hydrothermal route, involving precipitation of La(OH)$_3$ followed by amorphous IrO_x growth, with selected samples calcined at 450 °C to form IrO_2. Phase and elemental composition were analyzed by XRD, XPS, and FESEM-EDX. OER activity and stability were evaluated in 0.5 M H_2SO_4 using LSV, Tafel analysis, ECSA, and 6 h accelerated degradation tests combined with ICP-OES. Single-cell tests were performed on 5 cm^2 electrodes at 80 °C.

3. Results and Discussion

Ir-La catalysts with different atomic ratios were synthesized and systematically characterized. Comparison of bulk- and surface-sensitive elemental compositions (EDX and XPS) confirms the formation of a core-shell structure, as visible from the iridium enrichment on the surface. This is consistent with the two-step synthesis strategy designed to maximize Ir utilization [2].

XRD reveals a mixed amorphous-crystalline nature for the as-prepared catalysts, with La(OH)$_3$ reflections visible and the IrO_x shell predominantly amorphous. Upon calcination at 450 °C, crystalline IrO_2 phases emerge and partially dominate the diffraction pattern, making La-related features less distinct. FESEM images reveal sponge-like morphologies of aggregated nanoparticles, favoring high surface exposure. Electrochemical OER performance was evaluated by LSV and Tafel analysis in a three-electrode configuration under acidic conditions. The synthesized catalysts exhibit a cathodic shift in polarization curves compared to commercial IrO_2, resulting in lower overpotentials at 10 mA cm^{-2}, except for the calcined IrO_x_450 samples (Figure 1a). Among the compositions, La25 (η_{10} = 250 mV) and IrO_x (η_{10} = 251 mV) show the best activity, followed by La50, which achieves an overpotential of 269 mV. Tafel analysis confirms improved kinetics, with slopes of 40-45 mV dec^{-1} versus ~55 mV dec^{-1} for benchmark IrO_2. Calcination slightly reduces activity despite similar ECSA, suggesting that increased crystallinity modestly limits performance. Stability tests reveal a slight decrease in durability with increasing La content; however, all Ir-La catalysts retain higher OER activity than IrO_2, highlighting the beneficial effect of the core-shell architecture. Notably, PEM electrolyzer tests (Figure 1b) reverse the activity trend observed in half-cell measurements, with calcined samples outperforming the non-calcined catalysts. This trend can be attributed to the lower ohmic resistances measured by EIS, which are particularly relevant under device-operating conditions and arise from the enhanced electronic conductivity of crystalline IrO_2 formed upon calcination.



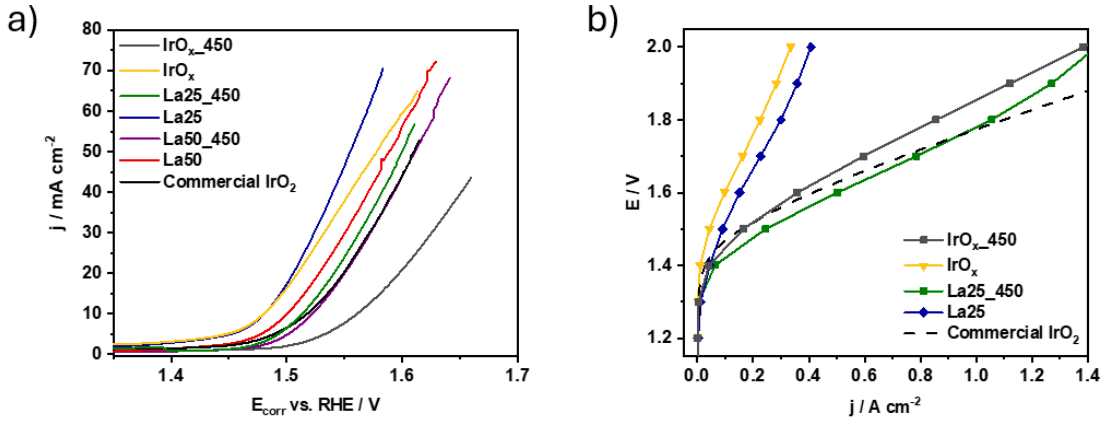


Figure 1. *a) LSV in 0.5 M H_2SO_4 using a three-electrode setup, and b) polarization curves recorded in a PEM cell.*

4. Conclusions

$La(OH)_3$-IrO_x catalysts were synthesized via a simple, green, and easily scalable hydrothermal route. EDX and XPS confirm a core-shell architecture, enabling reduced Ir content and optimized intrinsic activity through La incorporation. The catalysts deliver superior OER performance compared to commercial IrO_2 while maintaining comparable stability, supporting further validation in PEM water electrolyzers.

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CO_2-TO-METHANOL SYNTHESIS: EXPERIMENTAL, MODELING, AND PROCESS ASSESSMENT OF Cu-, In-, AND ZnZr-BASED CATALYSTS - (C093)

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Keywords: CO_2 hydrogenation, Methanol, Catalyst, Reactor modelling, Process simulation

1. Introduction

Methanol from CO_2 and renewable H_2 offers a route to decarbonize chemicals and energy. Industry relies on $Cu/ZnO/Al_2O_3$ (CZA) catalysts (TRL 9), originally for syngas. CZA works for CO_2 hydrogenation but suffers water-induced deactivation. To address this limitation, alternative indium oxide– (IZ) and zinc–zirconia–based (ZZ) catalysts have been proposed. Designed for CO_2 hydrogenation, they show improved water tolerance but remain at low technological readiness levels (TRL 4–5). Given this mismatch in TRL, a systematic and quantitative assessment under comparable production conditions is still lacking. Multiscale modeling and process-oriented methods are needed to assess how these novel catalysts perform versus industrial CZA at the same technological and process level.

2. Materials and Methods

CZA, IZ, and ZZ catalysts were synthesized by coprecipitation, characterized, and tested in a fixed-bed reactor in representative conditions (45-90 barg, 160–400°C, $H_2/CO_2 = 3$, GHSV = 4000-8000 h^{-1}). Full scale reactor behavior was assessed using literature kinetic models [1,2,3] via pseudo-homogeneous models in gPROMS® able to describe axial and radial temperature profiles, while process simulations were carried out using Aspen Plus® V11.

3. Results and Discussion

The kinetic models implemented for Cu- and In-based catalysts were successfully validated against experimental data (experimental validation for the $ZnO–ZrO_2$ system is currently ongoing), showing excellent agreement between simulations and experiments (Figures 1A and 1B). The CZA, IZ, and ZZ catalysts were synthesized, characterized, and tested in a lab scale fixed-bed tubular reactor. Products were quantitatively analyzed via online and offline GC analysis. Each catalyst family exhibits a distinct optimal temperature window: 220–280°C for CZA catalysts, 280–320°C for IZ systems, and 300–340°C for ZZ. Notably, In- and Zn-based catalysts can effectively suppress the reverse water–gas shift reaction, leading to increased methanol yields at high temperatures. Space–time yield (STY) values under reference conditions are 0.191 gMeOH/h/gcat for CZA, 0.116 for IZ, and 0.089 for ZZ. Given the well-known susceptibility of CZA catalysts to water-induced deactivation, achieving comparable productivity with more water-resistant systems represents a key objective; therefore, a sensitivity analysis on GHSV was performed and optimal conditions enabling STY values comparable to CZA systems were identified. The simulation of the entire process loop -level assessment (Figure 1C), performed for a small-scale industrial plant (reference size150 ton/day, 50 bar, feed from pure H_2/CO_2 stream), shows that the substitution of CZA with either IZ or ZZ catalyst cause a reduction in the produced methanol of about 30% , mainly due to lower per-pass conversions despite the higher reactor temperatures, leading to higher recycle ratios.



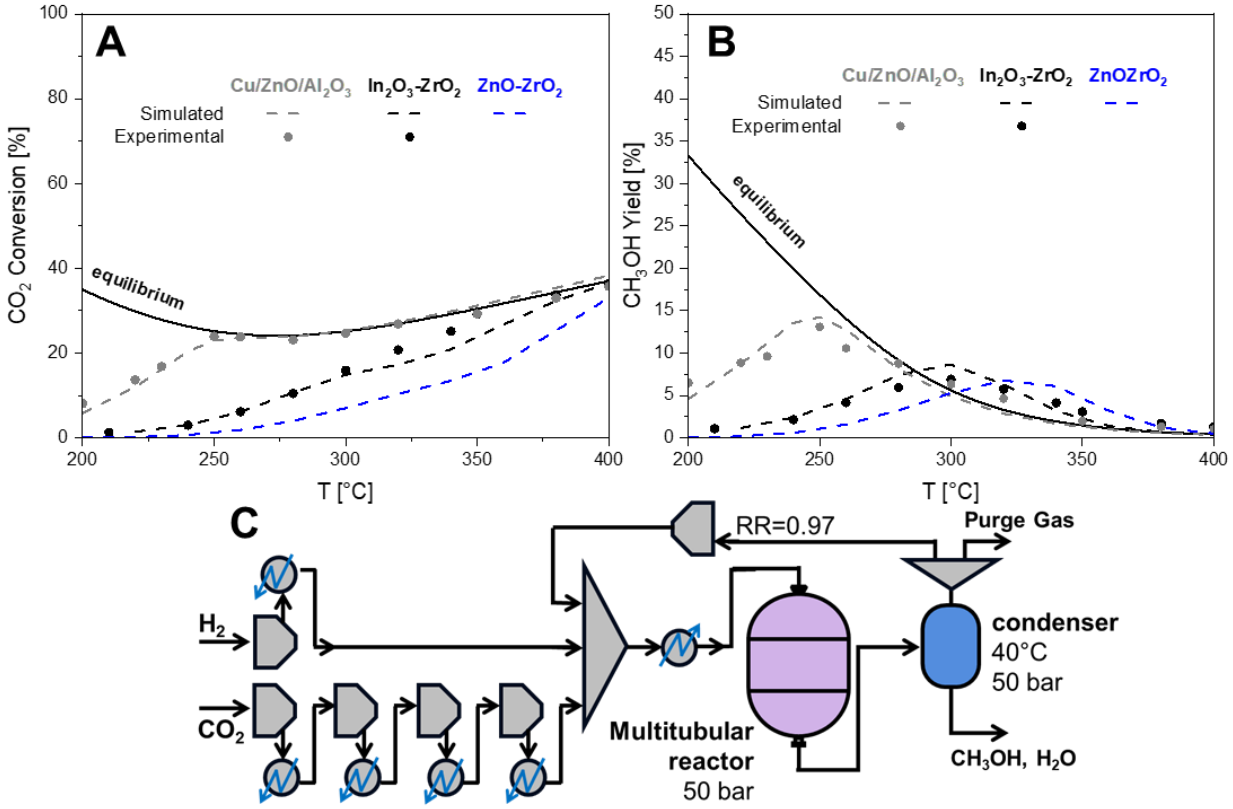


Figure 1. Simulated and experimental CO_2 conversion (A) and CH_3OH yield (B) for the three catalysts. Layout of the simulated small-scale methanol process (C).

4. Conclusions

This work provides a quantitative comparison of $Cu/ZnO/Al_2O_3$, $In_2O_3–ZrO_2$ and $ZnO–ZrO_2$ catalysts for CO_2 to methanol synthesis by integrating experimental validation, reactor modeling and process simulation. The results highlight the need for catalyst–process co optimization and evaluation of mixed feeds for realistic deployment, while showing that innovative water resistant systems still underperform conventional Cu catalysts.

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GASIFICATION OF PLASTIC WASTE WITH OXYGEN AND STEAM IN A LARGE PILOT SCALE GASIFIER - (C094)

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Keywords: Gasification, Fluidized Bed Gasifier, Hydrogen, Hot Syngas Cleaning, Tar Cracking.

1. Introduction

Worldwide, plastic waste management through mechanical recycling often results in downcycling, particularly when applied to mixed plastic waste (MPW), which consists of multilayer packaging and heterogeneous polymer mixtures. This inadequate management is the main reason for the low global plastic recycling rate (approximately 9%) with only 10% of plastics being recycled more than once[1], leading to the uncontrolled dispersion of contaminants. In this alarming context, advanced autothermal steam-oxygen gasification technologies aimed at hydrogen production represent a promising solution.

2. Materials and Methods

Our pilot-scale, FABER (Fluidized Air Blown Experimental gasification Reactor) is a bubbling fluidized bed gasifier (BFBG), schematically shown in **Errore. L'origine riferimento non è stata trovata.**. It has a total height of 4.7 m and an internal diameter of 0.489 m, sizes selected to minimize scale effects and ensure transferable results to commercial scale. The gasifier operates with a maximum thermal input of 400 kW and can be supplied with different fluidizing/gasifying agents (air, oxygen, steam, carbon dioxide, or their mixtures). Produced syngas is treated in a hot gas cleaning system for catalytic tar cracking.

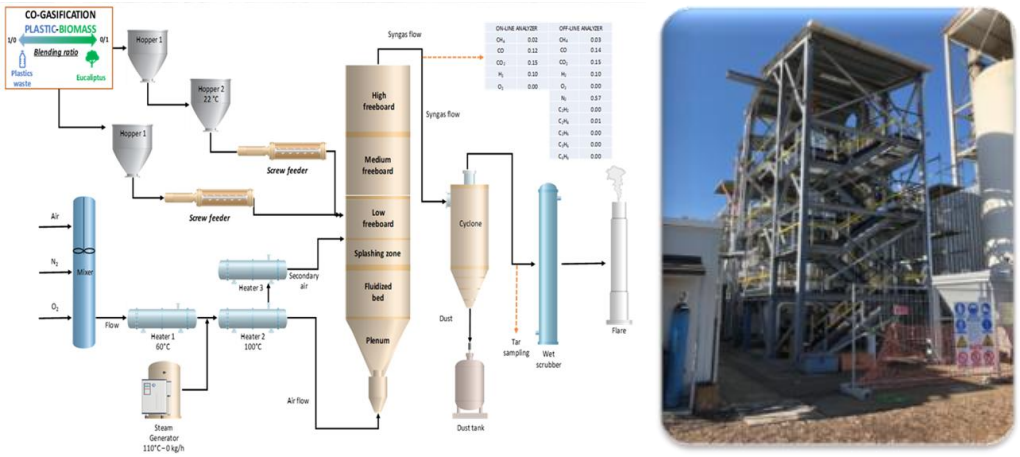


Figure 8 Pilot scale Bubbling Fluidized Bed Gasifier (BFBG).

3. Results and Discussion

This study presents gasification tests performed on mixed plastic wastes (MPWs) derived from separately collected municipal solid waste, using our pilot-scale fluidized bed gasifier. Experiments are conducted under steam and O_2-enriched air from 70% up to



100%. Obtained data allow investigation of the main operating parameters, such as equivalence ratio (ER) and steam-to-carbon molar ratio (StC). When air is employed as gasifying agent, ER is defined as the molar ratio between oxygen fed to the reactor and the amount theoretically required for the stoichiometric combustion of the feedstock. In contrast, autothermal steam-oxygen gasification requires control of an additional parameter: the steam-to-carbon molar ratio (StC), defined as molar flow steam divided by the molar flow rate of carbon in the feedstock[3]. Temperatures on both bed and freeboard must be maintained with a specific operating window, bounded at the upper limit by reactor material constraints and at the lower limit by the extent required for complete gasification reactions.

When nitrogen is removed from the gasifying medium, its thermal moderation effect must be compensated by steam. The inlet steam-to-oxygen molar ratio (StO_2) was adopted instead of StC, as it highlights the crucial role of steam as thermal moderator[3]. Experimental campaign showed that ER and steam-to-oxygen (StO_2) are the key operating parameters, as they jointly control temperature profile within the reactor. Several tests were performed in the hot cleaning system (**Errore. L'origine riferimento non è stata trovata.**) using gamma-alumina as catalyst, to evaluate its effectiveness in reducing tar concentration.



Figure 9 Hot gas cleaning system.

4. Conclusions

This work investigates the autothermal gasification of mixed plastic wastes through experimental campaigns conducted in a large-scale bubbling fluidized bed pilot reactor. The gasifier was operated with steam and O_2-enriched air employing increasing oxygen fractions (70-80-90-100%), equivalence ratios in the range 0.21 up to 0.27, and steam-to-oxygen ratios between 2.5 and 4.5. Moreover, tar conversion efficiency through hot gas cleaning system was investigated. It reached approximately 80% resulting in enhanced hydrogen concentration in the purified syngas.

Acknowledgements

This work was carried out with the financial support of Integrated Project Technologies and final uses of hydrogen - LA 1.16 Hydrogen production from non-recyclable plastic waste through Fluidized Air Blown gasification (Phase 2) - funded by The Italian Ministry of Environment and Energy Security within the framework of the Research on the Electric System program, Research Plan 2025-2027

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VOLCANIC ASH AS SUSTAINABLE INORGANIC SUPPORT FOR SUPERCAPACITORS ELECTRODES - (C095)

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Keywords: Volcanic ash, supercapacitors, size control, inorganic support

1. Introduction

The rapid deployment of sustainable energy technologies requires electrochemical energy storage systems based on low-cost and environmentally friendly materials. Supercapacitors are key devices due to their high power density and long cycle life, but their electrodes often rely on Critical Raw Materials or energy intensive nanocarbons [1][2]. This work explores volcanic ash, a naturally abundant and underutilized material, as an inorganic support for sustainable supercapacitor electrodes. Although typically considered electrochemically inactive, volcanic ash can be engineered to enable charge storage. The study shows how particle size control and green hybridization can transform volcanic ash into a functional and sustainable component for energy storage.

2. Materials and Methods

Volcanic ash, ejected during the 2019 Etna eruption, was downsized by grinding and ball milling to nanometric size and polished by a treatment in HNO_3. Scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), X-rays photoelectron spectroscopy (XPS) and Raman spectroscopy were used. Cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) were adopted. Hybrid electrodes were prepared by mixing volcanic ash and reduced graphene oxide via a green hydrothermal process.

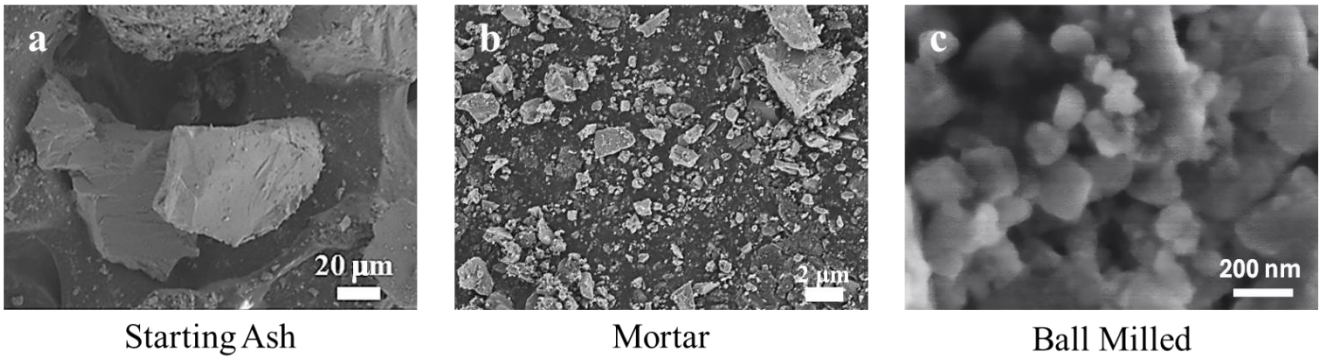
3. Results and Discussion

Figure 1 shows the particle size's reduction from about 150 μm for the starting ash (a) and 700 nm of the mortar case (b) to 100 nm of the ball milled one (c). Nearly rectangular cyclic voltammetry profiles (Figure 2 a) are obtained. The optimized volcanic ash reaches a specific capacitance of 25 F g^{-1} at 5 mV s^{-1}, five times higher than the value of 5 F g^{-1} for the pristine material (Figure 2 b), highlighting the intimate link between particle size, surface morphology, and electrochemical response. The increase in active surface area and improved ion accessibility appears to be key factors driving this enhancement. The capacitance enhancement is mainly attributed to particle downsizing, which improves electrolyte accessibility and shortens electronic transport paths, rather than to the formation of intrinsic porosity. Hybridization with reduced graphene oxide (rGO) further boosts performance. The stored charge was analysed as a function of rGO content, showing a clear increase up to 10 wt% followed by saturation. Remarkably, only 10 wt% rGO provides a charge storage comparable to pure rGO electrodes, demonstrating that the ash mainly acts as a low-cost high-surface inorganic scaffold rather than an electrochemically active component. This result indicates that a small amount of



conductive carbon is sufficient to build an efficient percolation network, significantly reducing the amount of expensive nanocarbon required.

Figure 1. SEM images of the initial ash (a), mortar (b) and ball milled (c) samples.



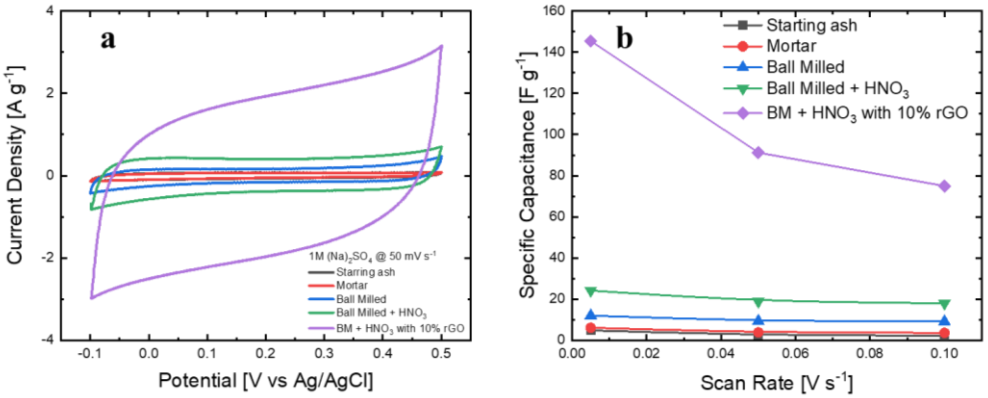


Figure 2. CV (a) and specific capacitance (b) of the different sized samples, of the Ball Milled samples after the chemical polish and of the final electrode with 10%wt of rGO.

4. Conclusions

This study shows that volcanic ash can be transformed into a low-cost, sustainable inorganic support for supercapacitor electrodes through particle size engineering and green hybridization. The approach reduces reliance on critical materials while maintaining competitive electrochemical performance. Thus showing a possible application and offering a novel and still underexplored route toward environmentally friendly energy storage materials offering a scalable, low-cost and sustainable route.

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BIO-FUNCTIONALIZED ELECTROSPUN MULTILAYER MEMBRANES AND SUSTAINABLE AQUEOUS ELECTRODES FOR LITHIUM-ION BATTERIES - (C096)

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Keywords: electrospinning, multilayer membranes, lithium batteries, carbon nanomaterials, sustainable electrodes

1. Introduction

The development of high-performance and sustainable components for lithium-ion batteries requires advanced separators and eco-friendly electrode formulations. Electrospun polymer membranes offer high porosity and tunable morphology, while carbon nanomaterials enhance conductivity. This work reports progress on PAN–PCL multilayer membranes functionalized with bio-based functional molecules and PEO-based systems, integrated with sustainable carbon-based electrodes and mucilage from Opuntia ficus-indica as a bio-based binder in aqueous electrode aiming to improve electrochemical stability, mechanical strength, and environmental compatibility

.

2. Materials and Methods

Electrospun PAN–PCL membranes functionalized with different biomolecules and PEO-based systems were produced and integrated into multilayer structures. Sustainable carbon-based materials, including MWNTs, graphene nanofibers, coffee-derived carbons, Opuntia ficus-indica as a bio-based binder were used for aqueous electrode formulations. Morphology was analyzed by SEM; electrochemical tests were performed in Li half-cells to evaluate conductivity and stability and thermal stability was analyzed by TGA.

3. Results and Discussion

PAN–PCL membranes differently functionalized with PEO-based systems and hyaluronic acid-based nanostructures were successfully realized. Systems containing PEO and hyaluronic acid nanostructures exhibited enhanced wettability and cohesion in multilayer architectures. Electrochemical testing in Li half-cells confirmed stability and suitability as separators. Cold lamination and laser texturing improved mechanical robustness while preserving fibrous morphology.



Carbon-based materials, including MWNTs, graphene nanofibers, and coffee-derived carbons, exhibited good conductivity and stable electrochemical response. Functional inks with $LiFePO_4$ and carboxymethyl cellulose (CMC)/ Opuntia ficus-indica as bio-based binders showed good dispersion, cohesion, and eco-compatibility.

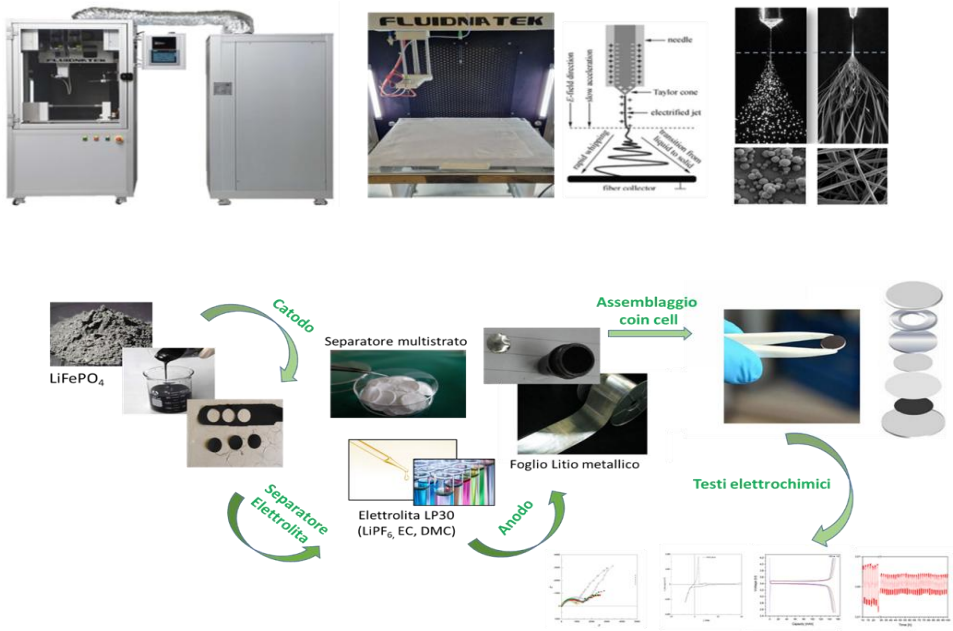


Figure 1. Integrated processing and characterization pathway of bio-functionalized multilayer separators and sustainable carbon-based aqueous electrodes for lithium-ion batteries

4. Conclusions

Functionalized PAN–PCL multilayer membranes demonstrate an a viable separator strategy compatible with bio-based functional molecules, with improved mechanical robustness enabled by lamination and laser texturing. In parallel, the integration of carbon nanomaterials and coffee-derived biochars with Opuntia-based aqueous binders supports low-impact electrode processing. Overall, these findings support the development of scalable, eco-friendly components for next-generation lithium-ion batteries.

Acknowledgements

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EFFECT OF PHOSPHORUS CONTENT IN Ni CATALYSTS SUPPORTED ON ACTIVATED CARBONS DERIVED FROM RESIDUAL BIOMASS IN CO_2 HYDROGENATION - (C097)

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Keywords: CO_2 hydrogenation, reverse water gas shift, nickel phosphide, catalysts, activated carbon.

1. Introduction

The hydrogenation of CO_2 offers a promising route to reduce fossil fuel dependency and greenhouse gas emissions. Nickel-based catalysts exhibit high activity for methane production through this process, while the use of nickel phosphides as active phases shift selectivity towards reverse Water Gas Shift (rWGS), at the cost of a huge decrease in activity. In addition, activated carbons (AC) provide several advantages as catalytic supports compared to conventional inorganic oxides, since they can be derived from lignocellulosic residues, show higher surface areas and have well-developed pore structures. However, their stability is compromised under oxidative atmospheres at high temperatures.

We recently found that the combination of nickel and nickel phosphides supported on biomass-derived AC modulates the catalytic activity of Ni-AC on steam reforming of pyrolysis liquids, while expanding the lifetime of the carbon support and therefore the stability of the catalyst [1]. In this contribution, we aim to extend these findings to Ni-AC catalysts for the CO_2 hydrogenation reaction, by studying the effect of the P-loading on their activity and selectivity towards methane or carbon monoxide. The P contents are kept under the stoichiometric Ni/P ratios so that mixtures of metallic nickel and nickel phosphides are obtained, expecting to combine the properties of both active phases in a novel catalyst.

2. Materials and Methods

Microporous activated carbon (S_{BET} = 1460 $m^2 \cdot g^{-1}$, V_{pore} = 0.51 $cm^3 \cdot g^{-1}$) free of any inorganic impurities was prepared by CO_2 gasification of an Organosolv lignin-derived char at 850 ºC for 6 h. The resulting support was loaded with ca. 10 wt.% Ni and varying phosphorus contents (using P/Ni ratios from 0.1 to 0.5 and indicated in the catalyst nomenclature) by wet co-impregnation using aqueous solutions of phosphoric acid and nickel nitrate, followed by a reduction treatment under 10% H_2 atmosphere at 600 ºC for 2 h.

The catalysts were characterized by XRF, XRD, XPS, TEM, TG, CO-chemisorption, CO_2-TPD, N_2 adsorption-desorption isotherms and TEM. Catalytic activity was evaluated at different reaction temperatures in a fixed-bed reactor using 100 mg of catalyst, with a feed containing 5 vol.% CO_2 in a total flow of 100 mL STP min^{-1} and maintaining an H_2:CO_2 ratio of 4:1, after in-situ reduction.

3. Results and Discussion

XRD analyses (Figure 1A) reveal the presence of metallic nickel in P-free Ni-AC catalyst. The incorporation of low amounts of P reduces the crystallite size (0.1P/Ni and 0.2P/Ni catalysts). At P/Ni ratios of 0.4 and above, the formation of nickel phosphides is



detected. The addition of phosphorus also extended the temperature onset for the gasification of the Ni-AC catalyst, as confirmed by TG analyses under CO_2 and H_2 atmospheres.

The P-free Ni-AC catalyst shows high CO_2 conversion with selective CH_4 production (>90%), approaching thermodynamic equilibrium at 450 °C (Figures 1B-C). The addition of P near to the stoichiometric ratio of $Ni_{12}P_5$ (0.4P/Ni) and Ni_2P (0.5P/Ni) caused a drastic decrease in methanation activity and CO_2 hydrogenation rate. Surprisingly, the addition of low amounts of P (0.1P/Ni 0.2P/Ni) significantly improved catalytic activity with respect to those of nickel phosphide, while keeping the selectivity towards the rWGS reaction close to 100%. The presence of phosphorus also expands the operational temperature window, and ensures high catalyst stability for TOS of 48h of reaction at 450 ºC, with only a 6% decrease in conversion and no significant change in selectivity.

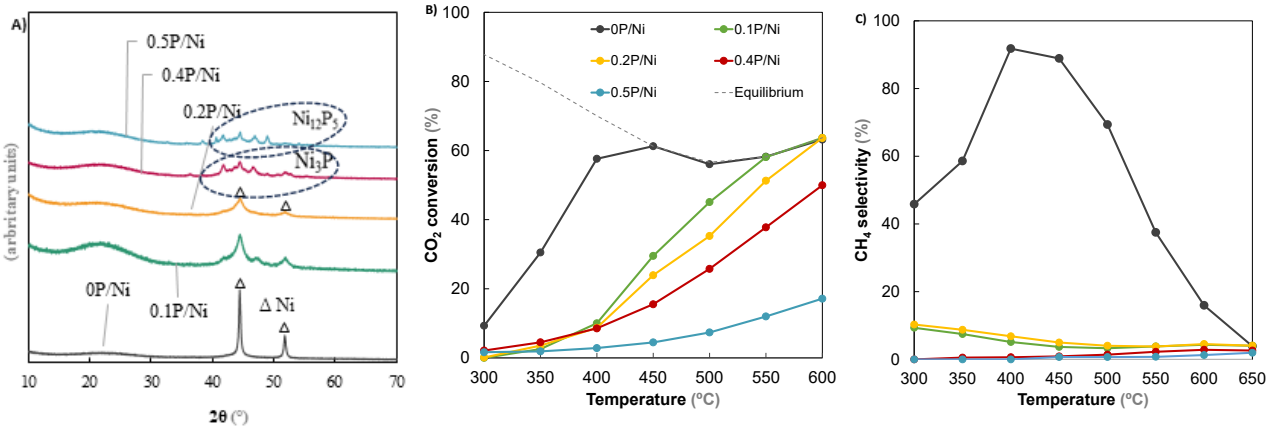


Figure 1. A) XRD of AC-Ni using different P-loadings. B) evolution of the CO_2 hydrogenation conversion as well as C) CH_4 selectivity at different reaction temperatures for the AC-Ni catalysts with different P loadings.

4. Conclusions

The addition of P in low amounts to biomass-based Ni-AC catalysts shifts the selectivity to rWGS, achieving CO selectivity over 95%, CO yield close to 40% at 450 ºC when a 0.1P/Ni ratio is used. These results pave the way for designing highly active and sustainable rWGS catalysts through straightforward and green methodologies.

Acknowledgements

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SOLAR HYDROGEN PRODUCTION VIA METHANE CHEMICAL LOOPING CYCLES USING A γ-Al_2O_3 SUPPORTED PEROVSKITE CATALYST - (C098)

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Keywords: Solar fuel, Chemical Looping Reforming, Oxygen Carriers, Perovskites, Directly Irradiated Fluidized Beds.

1. Introduction

The production of solar fuels using renewable energy is a key objective in achieving carbon neutrality. Chemical Looping Reforming (CLR) cycles powered by Concentrated Solar Thermal (CST) technologies offer a promising alternative to electrolysis for splitting H_2O and CO_2 to generate synthesis gas (H_2 and CO). In this context, the development of efficient oxygen carriers is crucial. Perovskite-based materials, particularly those modified through cathodic substitution, are being explored to enhance redox performance and stability in CL processes. In this work, an innovative material with chemical formula $La_{0.6}Sr_{0.4}Mn_{0.4}Fe_{0.6}O_3$, has been synthetized and CLR cycles tested and performed in conventional and unconventional fluidized beds [1].

2. Materials and Methods

The catalyst was prepared by impregnating γ-Al_2O_3 [2]. The γ-Al_2O_3 support enhanced the mechanical properties and characteristics of the material, making perovskites suitable for operation in a fluidized bed reactor. Isothermal cycles were conducted at different conditions. Each cycle includes: i) a reduction step with a mixture of CH_4 at 5% in N_2, during which supported perovskite particles are reduced to a $La_{0.6}Sr_{0.4}Mn_{0.4}Fe_{0.6}O_{3-\delta}$ state with the contextual production of CO/H_2; ii) an oxidation step with H_2O or CO_2, during which the catalyst active phase returns its original form and H_2 is produced; iii) a final step in air for complete catalyst reoxidation is performed even to oxidize carbon deposits if formed during step i). The system shown in Fig. 1A consists of a 10 mm quartz tubular fluidized bed reactor in which tests were conducted at different temperature conditions in H_2O splitting. Fig. 1B shows the solar experimental apparatus which is made of an unconventional fluidized bed reactor coupled with a sun simulator consisting of a Xenon lamp and an elliptical reflector. The reactor comprises of two concentrically assembled tubes connected to a conical receiver. The inner tube (riser) has an internal diameter of 10 mm and a length of 120 mm, while the outer tube has an internal diameter of 16 mm and a length of 70 mm (anulus). CO_2 splitting CLR tests were conducted in this setup using a 7 kWe nominal power.



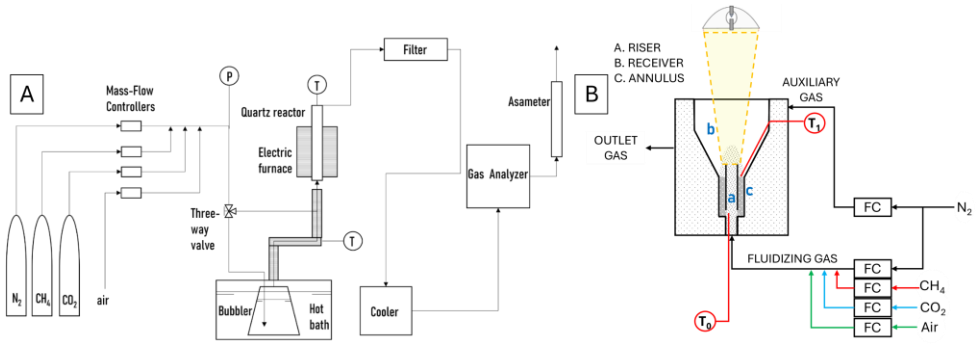


Figure 10. Experimental apparatus for conventional [A] and solar unconventional [B] fluidized beds.

3. Results and Discussion

The Fig.2 shows the typical concentration profiles in both conventional (A) and solar unconventional fluidized bed (B). The figure exhibits the three steps of the tests: i) methane reduction with the production of H_2, CO, CO_2; ii) water splitting for the Fig.2A, and CO_2 splitting for the Fig.2B; iii) air oxidation step.

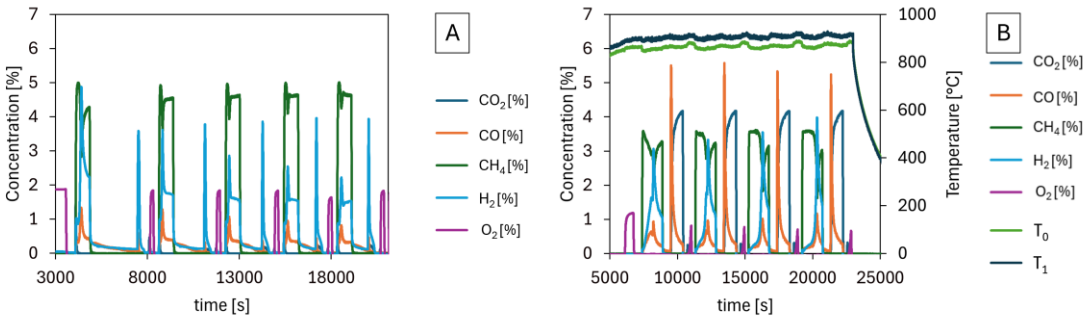


Figure 11. Gas concentration profiles in tests conducted in conventional [A] and solar unconventional [B] fluidized beds.

Table 1 shows the moles of H_2 produced for reduction step of each CLR cycle per gram of catalyst.

Conventional FB	Solar Unconventional FB
$mmolH_2/g_{LSMF.6}$	
13.99	10.59
10.71	9.66
9.29	8.84
8.80	8.56
8.27	-

Table 1. Produced moles per gram of LSMF.6 catalyst material, during the reduction step, in the two reactor configurations.



4. Conclusions

The study examines various experimental conditions to produce H_2 from methane assisted CLR using an innovative catalyst. The catalyst is also tested in a solar unconventional fluidized reactor.

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SERP METHANOL SYNTHESIS FROM CO_2/H_2: FROM EXPERIMENT TO SIMULATION TO OPTIMIZE AN INTENSIFIED PROCESS - (C099)

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Keywords: methanol synthesis, reaction-sorption, modeling, simulation.

1. Introduction

A strategy to overcome the thermodynamic limitations of the CO2 hydrogenation to methanol (whose yield at 80 bar and 230 °C is bound to 30%) lays in the employment of a sorbent that selectively adsorbs the products of the reaction, thus displacing the equilibrium temporarily rightward.[1] Molecular sieves like zeolites of Al-based MOF[2] are suitable sorbents for this application known as SERP (sorption enhanced reactive process).

Modelling of the SERP allows accessing non-trivially experimentally measurable pieces of information, for instance:

i. the effect of spatial distribution of catalyst and adsorbent inside the reactor (layering or mixing);

ii. the importance of the sorbent to catalyst mass ratio;

iii. the influence of the duration of each step of the cycle (reaction and purge)…

During this study, after an experimental campaign aiming to determine the kinetic, isotherm adsorption and experimental SERP to build models; all these aspects are in depth analyzed by the means of numerical simulations for optimization issues.

2. Materials and Methods

A lab scale fixed bed reactor of a diameter of 6 mm, is filled with commercial catalyst (CZA) and zeolite 4A. Isotherms adsorption was determined by breakthrough experiments for water, methanol, CO_2 and combination by 2 or 3 species at conditions closed to methanol synthesis. Different operating conditions for SERP experiments have been studied varying cycling time, ratio between catalyst and sorbent, temperature and pressure. The mass, energy and momentum balance equations of the model are integrated via Matlab solver; coupling gas phase, catalyst and sorbent exchange. Parameters like isotherms adsorption constants was re-adjusted from SERP experiments; SERP model parameters was validated based on our SERP experiments.

3. Results and Discussion

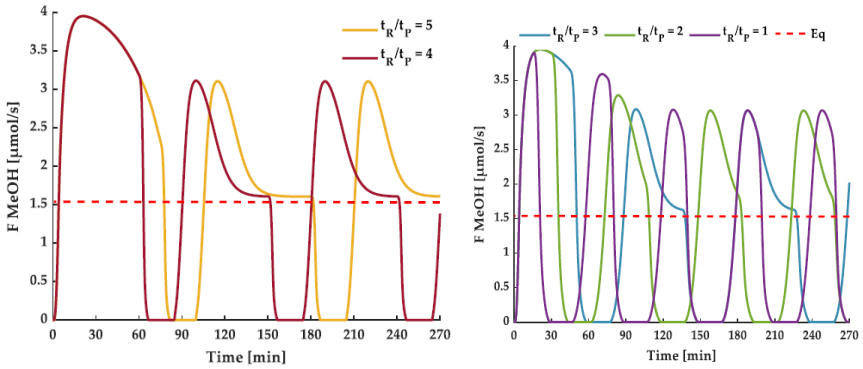


Figure 1. Effect of the reaction to purge timeslot on exiting MeOH flowrate. Left tR/tP = 5,4; right tR/tP = 3,2,1.



We were able to analyze different strategies for SERP optimization and the limits of this process. As visible in Figure 1 (operative cycles are carried out at 230 °C, 80 bar, with a Q = 125 NmL/min of reactants with a stoichiometric composition.), the gain of the process is represented by the overshoot in product concentration, that occurs in the reactive step; however when steady state is reached, a purge is required to restart the cycle. Therefore, the longer the reactive timespan, the more time the product flowrate will be equal to equilibrium, thus vanishing the advantage of working in non-equilibrium mode. Conversely, with too short productive steps, purge occurs too frequently, thus provoking the drop of the overall productivity. The best trade-off is represented by intermediate values that allow working as long as possible out of equilibrium, i.e. with the highest and broadest overshoot in concentration. Only finer indexes of performances, such productivity per volume of total solid or absolute yield will allow comparing different scenarios of such a multiphasic, complex process to foster the decision making in the frame of industrial, profit-demanding processes.

4. Conclusions

The maximum gain in Methanol productivity in the different scenarios of SERP based on 4A zeolites sorbent studied only by 26 % while in some situations SERP could be worse (-20 % in comparison with no sorbent) where the rapid saturation of the sorbent is one the most limitation of the SERP process.

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QUANTIFYING THE IMPACT OF WASTE HETEROGENEITY ON GASIFICATION PERFORMANCE: A DEEP LEARNING-BASED SURROGATE MODELING APPROACH FOR SYNGAS AND TAR PREDICTION - (C100)

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Keywords: Gasification, Process modeling, Waste valorization, Machine Learning, Waste-to-Value

Abstract: The conversion of heterogeneous waste streams (e.g., RDF, plastic-biomass blends) into liquid biofuels representsa strategic pathway for the circular economy [1]. However, the viability of downstream biorefinery processes (such as Fischer-Tropsch or Methanol synthesis) is strictly dependent on maintaining specific syngas quality standards, particularly the H2/COratio and low tar content, which are challenging to guarantee given the inherent compositional variability of waste feedstocks [2]. Exploring the vast multidimensional operational space to match diverse waste inputs with strict output targets is computationally prohibitive using solely rigorous mechanistic models. To bridge this gap, this work proposes a Deep Learning-based surrogate model of a Bubbling Fluidized Bed (BFB) gasifier. A rigorous steady-state 1D phenomenological model, accounting for two-phase hydrodynamics and detailed heterogeneous kinetics, was first developed to serve as the ground truth. This physics-based solver was utilized to generate a high-fidelity synthetic dataset by systematically perturbing feedstock characteristics (proximate and ultimate analysis) and operating conditions, effectively mapping the non-linear response of the reactor to waste heterogeneity. A Deep Neural Network (DNN) was then trained on this dataset,achieving high predictive accuracy ($R2 > 0.95$) with negligible computational cost. The surrogate model was subsequently deployed to perform a global sensitivity analysis, identifying the specific operational windows required to tune the syngas composition for biofuel applications. The results demonstrate how the model can rapidly determine optimal feedstock blending strategies to maximize the yield of useful synthesis gas while minimizing tar production, effectively decoupling process efficiency from the unpredictability of waste inputs.

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A REDUCED-PHYSICS 3D CFD MODEL FOR FIELD-DRIVEN DESIGN OF TPMS FLOW FIELDS IN PEMFC BIPOLAR PLATES - (C103)

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Keywords: Laser Powder Bed Fusion (LPBF), Triply Periodic Minimal Surface (TPMS), PEMFC performance

Bipolar plates govern reactant delivery, water and thermal management, electrical conduction and structural support in PEM fuel cells. Their flow-field design, however, introduces pressure losses that raise balance-of-plant power — notably for air supply — and reduce net system efficiency [1]. The design problem is therefore one of balancing pressure loss against adequate and uniform reactant availability. Manufacturing route and cost are equally constraining, as scalable, high-yield fabrication ultimately governs €/kW and the transition from prototypes to volume production [2]. Laser powder bed fusion (LPBF) is attractive on both counts, unlocking flow-field architectures that are difficult or impractical to realize by conventional forming or machining [3]. Triply periodic minimal surfaces (TPMS) are a representative example: three-dimensionally periodic architectures of zero mean curvature that partition space into interpenetrating, continuous channel networks, offering high specific surface area and transport properties tunable through a small set of geometric parameters.

That same parameterisation — unit-cell size, wall thickness, level-set offset, spatial gradation — generates a design space far too large to explore by building and testing candidate plates one at a time, making simulation the natural screening tool. A fully MEA-resolved model (GDL, MPL, catalyst layer, membrane, two-phase transport and electrochemistry) is, however, computationally prohibitive for parametric geometric studies and introduces parameters that cannot be identified independently from cell-level data, so that predicted differences between geometries may reflect parameter choices as much as geometry itself.

This work takes the opposite approach: only the flow-field fluid domain is resolved, while the entire through-plane transport of the GDL/MPL/CL stack collapses into a single effective coefficient acting at the electrode-facing boundary. The model is cheap enough for parametric screening and, being spatially resolved, is used not only to rank geometries but to redesign them — the information extracted from the oxygen field over the electrode surface is fed back into the geometry generator as a driving scalar field, locally grading the TPMS unit cell where the simulation predicts starvation. The workflow is demonstrated on a gyroid flow field, progressively graded and re-simulated, and benchmarked against a conventional multi-pass parallel-channel serpentine.

2. Materials and Methods

The computational domain is the cathode flow-field fluid volume. The air stream is treated as a steady, isothermal, incompressible single-phase flow governed by continuity and the Navier–Stokes equations:

$$\nabla \cdot u = 0 \tag{1}$$

$$\nabla \cdot (\mathrm{u} \otimes \mathrm{u}) = -\nabla \mathrm{p} + \nabla \cdot (\nu \nabla \mathrm{u}) \tag{2}$$



With p the kinematic pressure and ν the kinematic viscosity of the mixture at the operating conditions. Oxygen is transported as a molar concentration field (c) convected by the resolved velocity field:

$$\nabla \cdot (u\, c) = \nabla \cdot (D_{O_2}\, \nabla c) \tag{3}$$

Where D_{O_2} is the diffusivity of oxygen in the air mixture. No source term appears in the interior of the domain: the whole electrochemical consumption enters as a boundary flux, which is the defining feature of the reduction. At the inlet, a uniform mass-flow rate is set by the applied current density and cathode stoichiometry λ, together with the inlet oxygen concentration c_{in} of air at the operating temperature and pressure. The outlet is prescribed at static pressure while plate and land walls are no-slip and impermeable, with zero normal flux of c.

The GDL, MPL and CL are not meshed, their combined effect enters solely through an effective mass-transfer coefficient k_m applied at the boundary faces in contact with the electrode. The boundary flux and the lumped coefficient are defined as:

$$-D_{O_2} \left.\frac{\partial c}{\partial n}\right|_i = N_i, \qquad \frac{1}{k_m} = \frac{A_{GDL}}{A_{act}} \sum_i \frac{L_i}{D_{eff,i}}, \qquad D_{eff} = \frac{\varepsilon}{\tau} D \tag{4}$$

Where N_i is the molar flux consumed at face i, transmitted through the unresolved GDL/MPL/CL stack, A_{GDL}/A_{act} the ratio of the electrode-facing area to the active area, L_i and $D_{eff,i}$ are the thickness and effective diffusivity of each layer, ε and τ the porosity and tortuosity. Each electrode-facing face consumes a patch-wide molar flux N^*, limited by the local transport capacity of the stack. Under galvanostatic operation the total consumption is constrained by the applied current, which closes the problem for the single unknown N^* with a mixed Robin-Neumann boundary condition:

$$N_i = \min(k_m c_i, N^*), \qquad \sum_i N_i A_i = \frac{j A_{act}}{4F} \tag{5}$$

The formulation implies zero-order kinetics in oxygen and requires no kinetic parameters. Where the transport ceiling is not binding the local consumption is uniform by construction, so the model predicts oxygen and consumption-flux fields rather than current distribution.

Geometries are ranked by the inlet-to-outlet pressure drop Δp, a proxy for the parasitic blower power, together with four area-weighted metrics evaluated on the electrode-facing surface: the normalised mean surface concentration $\bar{c}/c_{in}$ defined as $\bar{c} = \sum c_i A_i / \sum A_i$; the normalised minimum c_{min}/c_{in}, indicating worst-case starvation; the coefficient of variation $\mathrm{CoV} = \sigma_c/\bar{c}$, with $\sigma_c = \sqrt{\sum (c_i - \bar{c})^2 A_i / \sum A_i}$, a scale-free measure of dispersion; the uniformity index $\mathrm{UI} = 1 - \sum |\, c_i - \bar{c}\, | \, A_i / (2\bar{c} \sum A_i)$, bounded in [0,1] and equal to unity for a perfectly uniform surface.

3. Results and Discussion

The TPMS flow field is a gyroid; a conventional multi-pass parallel-channel serpentine of equal active area (50 cm²) serves as reference. The oxygen concentration returned at the electrode surface is used as a design driver rather than only as a diagnostic: in a field-driven workflow a scalar field defined over the plate modulates the local



TPMS parameters at generation time — here the unit-cell size, which sets the local hydraulic diameter and hence the local flow resistance.

The baseline gyroid reveals a poorly supplied region at the center of the plate, indicating that the channel should be widened there to promote airflow. The driving field is accordingly discretized over the electrode surface into four zones, and then nine, each assigned a different unit-cell size, yielding a spatially graded TPMS. Evaluation metrics improve monotonically with the refinement of the driving field, evidence that the gain follows the field rather than an incidental geometric change. The graded design nevertheless does not reach the area-averaged surface concentration of the serpentine, which remains superior in reactant delivery. That superiority, however, is bought at a pressure drop roughly an order of magnitude higher.

4. Conclusions

A three-dimensional CFD model of the flow field, coupled to a reduced transport closure that collapses the GDL, MPL and catalyst layer into a single microstructurally traceable coefficient, was used to characterise TPMS flow-field geometries at a preliminary design stage. Because the closure introduces no kinetic parameters, the differences observed between geometries are attributable to geometry and lumped transport alone.

The resolved oxygen field was then used prescriptively rather than only diagnostically. Feeding it back as a driving scalar field and grading the local gyroid unit-cell size in the regions the baseline simulation identified as under-supplied, improved the transport metrics monotonically with the refinement of the field. This establishes field-driven design as a practical route to correcting spatially localized deficiencies that an integral performance metric cannot expose, and one that exploits the parametric freedom of TPMS architectures in a way a uniform unit cell cannot. The same workflow, however, returns a cautionary result about the architecture itself. Neither the baseline nor the graded gyroid matches the surface oxygen delivery of a conventional parallel-channel serpentine, indicating that the high specific surface area and low hydraulic resistance of TPMS flow fields do not translate directly into superior reactant distribution. That deficit is nevertheless incurred at a pressure drop roughly an order of magnitude lower, shifting the case for TPMS from cell-level reactant delivery to system-level parasitic-power savings.

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TRUE OR FALSE? THE THREAT OF FAKE SCIENTIFIC INFORMATION - (C104)

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Keywords: fake claims, retraction, renewable energy, misinformation, media, scientific literature

1. Introduction

As scientists, we have a serious social and ethical responsibility to call out misinformation and disinformation that is spread through the media, internet, social networks and the scientific literature[1,2]. False information in the media and social networks creates confusion in the minds of the public and may also discredit the scientists involved. Chemistry plays a central role in addressing renewable energy and related climate change mitigation. Consumers (ie the public in general) are the beneficiaries of these chemical endeavors in relation to sustainable energy generation, but the false information discredits the importance of chemistry and chemical manufacturing for society in general.

Misinformation as well as deliberate disinformation is used to falsely pursue political and commercial agendas, without due consideration of sustainability issues and addressing climate change. This presentation will provide examples of false chemical and related information in both the public arena as well as the scientific literature.

2. Materials and Methods

An overview of current literature and media reports was undertaken, focusing on the last five years and drawing pertinent examples from these sources. Information was also sourced from a number of reputable online databases that identify retracted, and dubious scientific research[3]. These are freely available to consult.

3. Results and Discussion

This study revealed a large volume of scientific literature detailing falsified information and many media reports containing incorrect information. False reports and misinformation related to climate change and renewable energy have impeded efforts to address renewable energy developments that are vital for fighting climate change. Public support, influencing political decisions and policies are essential for supporting renewable energy efforts. Conflicting information from different sources has resulted in people often doubting scientific facts and that their judgement is often based on a combination of education, social and cultural influences[4]. AI tools also provide the means for generating and structuring convincing falsified manuscripts, often difficult to detect[3].

4. Conclusions

A change in rhetoric has occurred, whereby casting direct doubt on climate change evidence has transgressed to suggesting that climate solutions are ineffective, risky and not viable[5]. There are many reasons for the proliferation of false scientific information being spread through different communication channels. Pressure to publish for career advancement, pressure to obtain funding and poor science are key reasons for falsified or misleading scientific publications. In the public media, political agendas, commercial interests, poor journalism and ignorance are responsible for false information. Ethical scientists need to identify and combat bad science and wrongful information which delay addressing global challenges and threatened planetary boundaries.



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EXPLORING THE EFFECT OF CE AND CU DOPING ON Ni/MgO CATALYSTS FOR CH_4 DRY REFORMING AND CH4 ACTIVATION - (C105)

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Keywords: Ni-MgO catalysts, Ce and Cu promotion, basic properties, CH_4 dry reforming, coke formation

1. Introduction

Dry reforming of methane (DRM) converts CH_4 and CO_2 into syngas, simultaneously mitigating greenhouse gas emissions and providing versatile feedstock for fuels and chemicals. Ni-based catalysts offer a cost-effective route for the reaction but are prone to rapid coking, sintering, and deactivation. Basic supports such as MgO improve Ni dispersion and mitigate carbon deposition via strong metal-support interactions,[1] though these interactions can limit Ni reduction and lower activity. Promoter doping provides a strategy to balance reducibility, basicity, and carbon tolerance.[2-3] This study systematically explores Ce and Cu promotion of Ni/MgO catalysts, assessing their individual and combined effects on methane dry reforming, methane cracking and coking resistance. Detailed characterization to elucidate structure–activity relationships have been performed.

2. Materials and Methods

MgO and doped MgO supports with wt% compositions Ce(18%)MgO, Cu(8%)MgO, Cu(18%)MgO, Ce(9%)MgO and Cu(9%)Ce(9%)MgO were synthetized via hydrothermal method using Pluronic P123 as surfactant and calcined at 600 °C, then, Ni was deposited by wetness impregnation method with a loading of 10 wt% and again calcination was performed at 600 °C. Catalytic tests were performed over catalysts previously reduced under H_2 (5 % in He, 50 mL/min) at 800 °C for 1 h with a ramp rate of 10 °C/min. The feed (15 % CH_4 + 15 % CO_2 in N_2) flowed at 100 mL/min (STP), corresponding to a WHSV of 60,000 mL g^{-1} h^{-1} or by flowing only 15 % CH_4 in N_2 for CH_4 cracking. Characterizations on fresh and/or used catalysts were carried out by XRD, H_2-TPR, CO_2-TPD, Raman, TGA, TEM analyses.

3. Results and Discussion

XRD and H_2-TPR analyses were carried out to study the structural and reduction properties of the Ni-MgO based catalysts. It was shown that Ni^{2+} was mainly incorporated into the MgO lattice as a Ni–Mg–O solid solution, ensuring high dispersion and strong metal–support interaction. After reduction, Cu-free samples formed metallic Ni^0, while Cu-containing catalysts produced Ni–Cu alloy phases whose composition depended on Cu loading. Promoters reduced the MgO surface area likely due to partial pore blocking. Subsequent Ni deposition did not cause significant changes in the textural properties compared to the corresponding supports.

Ce addition enhanced reducibility of surface Ni species and oxygen mobility, significantly increased surface basicity and CO_2 adsorption. The highest CO_2 uptake was observed for the Cu–Ce co-promoted catalyst, suggesting synergistic effects that likely enhance the formation of oxygen vacancies. In contrast, high Cu loading (18wt%) decreased the surface basicity, likely due to modifications at the metal–support interface that limit the number of MgO-derived basic sites. All catalysts were active in DRM



between 450 and 800 °C, with CH_4 conversion increasing with temperature. Ni–Ce(18%)MgO and Ni–Cu(18%)MgO reached >95% conversion above 700 °C. The H_2/CO ratio approached unity at high temperature, notably Ce-containing catalysts achieved near-stoichiometric values at relatively low temperatures. Stability tests at 650 °C (up to 80 h) revealed that Ce-promoted catalysts exhibited the best durability, with only 8–11% deactivation and limited carbon formation. In contrast, Cu-only catalysts showed rapid deactivation and higher coke accumulation, especially ordered graphitic carbon. The co-promoted system showed intermediate stability, with Ce partially suppressing carbon but not fully compensating for Cu effects. Overall, catalyst performance was governed by the balance between CO_2 activation and methane activation/alloy effects.

4. Conclusions

This work clarifies the structure–performance relationships of Ni/MgO catalysts in DRM. Ce improved basicity and oxygen mobility, enhancing CO_2 activation, reducing coke, and ensuring stable operation with near-unity H_2/CO. Conversely, Cu forms Ni–Cu alloys that promote preferential methane activation and cracking with high carbon coke deposition and deactivation in DRM tests. Overall, Ce-promoted catalysts offer the best balance of activity and durability.

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FABRICATION OF STRUCTURED COMPOSITE PHOTOCATALYTIC MEMBRANES: FROM HOLLOW FIBER ENGINEERING TO REACTOR IMPLEMENTATION IN WATER TREATMENT - (C107)

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Keywords: structured photocatalytic membranes, hollow fiber photocatalysts, TiO_2 nanocomposites, Photocatalytic membrane reactors, water treatment

1. Introduction

Photocatalytic materials, predominantly based on TiO_2, have attracted significant attention for environmental remediation, especially in water treatment. However, powdered catalysts face separation and recovery limitations that hinder large-scale application [3]. Recent research therefore focuses on immobilizing photocatalysts within structured composite, mixed matrix membranes (MMMs) and fibrous systems to improve stability, reusability, and process efficiency. Building on our group's expertise in hollow fiber engineering, membrane functionalization, and photocatalytic membrane reactor integration, this work presents fabrication and implementation case studies, highlighting mechanical robustness, synergistic photocatalysis-filtration performance, and long-term operational stability in advanced water treatment systems [2-5].

2. Materials and Methods

Hollow fibers were prepared by wet-spinning of TiO_2-alginate mixtures, followed by cross-linking and thermal treatment under air or N_2, yielding robust ceramic photocatalytic fibers [3]. Alginate, a non-toxic, biocompatible, biodegradable biopolymer, served as the matrix [3, 5]. Cu/Ca decoration and pyrolytic carbon enhanced functionality [3]. Complementary PVDF-based photocatalytic fibers and wash-coated ceramic monoliths were evaluated in photocatalytic filtration and reactor systems for water treatment [4].

3. Results and Discussion

Figure 1 summarizes the structural, functional, and operational performance of the developed systems. The structured photocatalytic membranes exhibited uniform hollow fiber morphology with well-defined lumen structure and high surface area. The fibers exhibited hierarchical bimodal porosity arising from nanoparticle packing and fiber structuring, while thermal processing preserved anatase crystallinity, contributing to enhanced charge transport and photocatalytic efficiency. Thermal treatment strongly influenced textural properties. Pyrolysis under inert atmosphere generated residual carbon, enhancing mesoporosity and pollutant adsorption capacity. Copper decoration resulted in well-dispersed Cu/CuO nanoparticles, promoting charge separation and suppressing electron-hole recombination. The nanocomposite fibers demonstrated superior photocatalytic



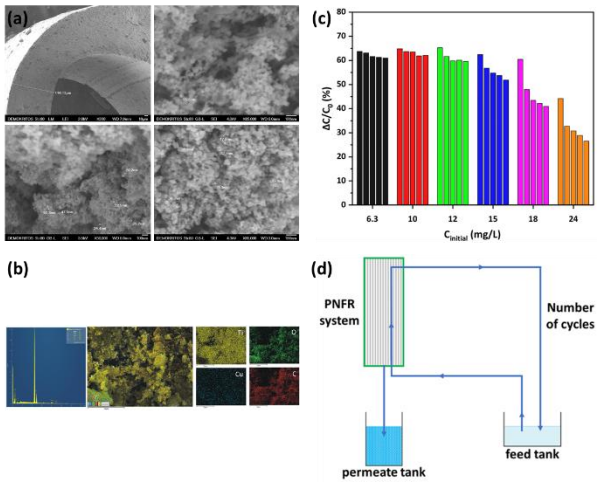


Figure 1. Structured TiO_2 photocatalytic membranes: (a) HF morphology [3], (b) nanoparticle mapping [3], (c) rejection performance [5], (d) reactor integration for continuous water treatment [4].

activity, achieving up to 70% degradation of methyl orange under UV irradiation, with adsorption contributing synergistically to pollutant removal. Oxygen availability significantly influenced degradation kinetics through reactive oxygen species generation, while O_2-depleted conditions favored initial adsorption. The ceramic fibers

maintained structural integrity, resistance to attrition, and stable performance over repeated and multiple cycles. Beyond batch operation, structured photocatalysts were integrated into photocatalytic membrane systems, including wash-coated ceramic multi-channeled monoliths and PVDF-based photocatalytic hollow fibers. Their incorporation into a pilot photocatalytic nanofiltration reactor enabled simultaneous filtration and degradation of pesticide contaminants under continuous flow, demonstrating high water recovery and operational feasibility for advanced wastewater treatment applications.

4. Conclusions

Structured TiO_2-based photocatalytic membranes were successfully fabricated via alginate templating and thermal conversion. Metal nanoparticle decoration and residual carbon enhanced adsorption, charge separation, and photodegradation efficiency. The mechanically robust hollow fibers demonstrated stable cyclic performance, while integration into photocatalytic membrane reactors validated their potential for continuous-flow operation and sustainable large-scale water treatment applications.

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KAPMEMLYSE:INTEGRATING CAPILLARY FEEDING AND AEM TECHNOLOGY FOR EFFICIENT, NOBLE METAL FREE HIGH PRESSURE WATER ELECTROLYSIS - (C114)

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Keywords: Capillary-fed water electrolysis, Anion exchange membrane electrolysis, Gas diffusion electrodes, High-pressure green hydrogen, Noble-metal-free catalysts

1. Introduction

KapMemLyse is an interdisciplinary research initiative of TU Ilmenau and Fraunhofer IKTS that aims to develop a new generation of water electrolyzers. Anion-exchange-membrane electrolysis (AEMEL) promises PEM-like performance with earth-abundant catalysts but is still limited in stability and pressurized operation [1, 2]. The capillary-fed cell of Hodges et al. enables bubble-free operation and very high efficiency yet uses a porous separator that prevents differential-pressure operation and degrades gas purity [3]. KapMemLyse will realize a capillary-fed AEM electrolyze with pressure-stable AEMs and capillary gas-diffusion electrodes and demonstrate a five-cell stack (~200 W) up to 10 bars using tightly coupled multiscale simulations and experiments.

2. Materials and Methods

The following cell-setup was used. The anode consisted of two or three layers. The first layer is the metallic gas diffusion layer (GDL), and the second layer can be a catalyst coated substrate (CCS) or a porous transport layer (PTL). The third layer is a catalyst coated membrane (Nickel @ PES) if the second layer is a PTL (Nickel foam). The cathode consisted of a commercial carbon-based GDL with a micro porous layer coating on it. This carbon GDL is coated by drop-casting or spin-coating method with NiMo. As capillary membrane the same porous polyether sulfone (PES) with 8 µm average pore diameter as in the Hodges paper [3] was used.

3. Results and Discussion

The first objective of the project was the development of gas diffusion electrodes (GDEs) for the anode and cathode, which are supplied with reactants via the capillary membrane. Several cell configurations incorporating capillary membranes were evaluated. The PES-Cell served as the reference, whereas the IonoPES-Cell represented the optimized configuration and exhibited a substantially lower cell voltage at 400 mA cm^{-2} (2.2 V) than the reference (2.8 V). The reference cell employed a metallic gas diffusion layer (GDL) and a catalyst-coated-substrate (CCS) on the anode, and a carbon GDL with a catalyst coating on the cathode. In contrast, the IonoPES-Cell featured a modified anode, consisting of the metallic GDL, a porous transport layer (PTL), and a catalyst-coated PES. This altered architecture led to a pronounced improvement in electrochemical performance, indicating that the anode GDE is significantly more active and/or facilitates more efficient gas bubble removal than the reference anode. The cathode of the IonoPES-Cell also showed enhanced activity (1.48 V at 400 mA cm^{-2}) compared to the reference cathode (2.25 V), which is attributed to differences in catalyst layer formulation. The reference cathode contained a higher ionomer content (20 wt% Fumion) than the IonoPES cathode (0.4 wt%), which more strongly obstructs gas transport because the ionomer blocks the gas pathways within the GDL. Nevertheless, the IonoPES cathode will be further optimized in order to increase its activity to a level comparable to that of the IonoPES anode.

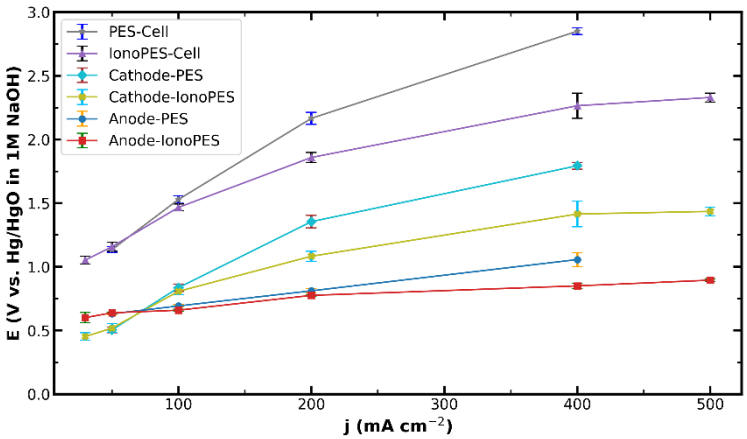


Figure 1: Current density plot of PES-Cell setup and their anode, cathode, and separator (PES) contributions.

4. Conclusions

Capillary-fed AEM cells with IonoPES-based electrodes show markedly improved performance, reducing cell voltage from 2.8 to 2.2 V at 400 mA cm-2 via optimized anode architecture and low-ionomer cathodes. Ongoing work will further enhance cathode activity and integrate these GDEs into high-pressure, noble-metal-free AEM stacks.

Acknowledgements

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WATER-BASED EXTRUDED LFP AND NMO ELECTRODES FOR SUSTAINABLE SIB AND NIB - (C115)

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Keywords: LFP, NMO, Electrode, Extrusion,

1. Introduction

Lithium- and sodium-ion batteries rely on slurry-cast electrodes processed with toxic, flammable organic solvents, which limit electrode thickness, recyclability and sustainability. This work develops and validates water-based pipe–slit extrusion of LFP and NMO electrodes with controlled porosity, high mechanical integrity and electrochemical performance comparable to state-of-the-art cast electrodes.

2. Materials and Methods

$LiFePO_4$ (Life Power®P2, Aleees A13, IBUvolt® LFP200) and $Na_{0.7}MnO_2$ (IBUvolt® NMO) cathode masses were formulated with carbon black (e.g. Ensaco 250P) and aqueous binders (Na-CMC or Li-PAA). Active material and carbon were dry-mixed in an Eirich R02E intensive mixer, then combined with binder solutions in Linden kneaders (LKS2/LKS5) for 1–6 h. Extrusion was carried out on a vertical VAQRS 35 vacuum extruder (35 mm screw, up to 300 bar) equipped with a round pipe-slit die (300–500 µm gap) and an integrated slitting and unfolding device, yielding unsupported green tubes that were slit and flattened into tapes. The LFP tapes were optionally calendared down to desired thickness. All electrodes were dried under controlled conditions, characterized by FE-SEM, porosity and XRD, and evaluated electrochemically in coin cells (EL-Cell PAT-Heater-4) using standard Na- or Li-ion electrolytes and Li/Na-metal anodes.

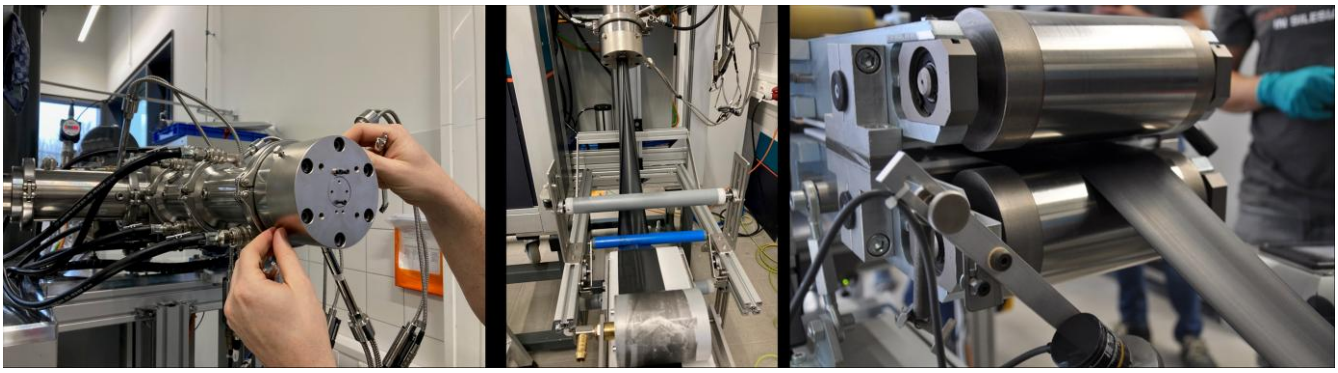


Figure 12 (left) extruder mouthpiece with pipe–slit, (middle) extruded electrode, (right) electrode after calandering

3. Results and Discussion

All three LFP powders could be processed successfully. LFP1 and LFP2 produced very homogeneous microstructures, while LFP3 led to a more structure-porous foil (**Errore. L'origine riferimento non è stata trovata.**). Green densities around 2.06–2.07 g/cm³ and open porosities 25–29 % were achieved. Extrusion of LFP with pipe–slit tooling was stable across several tool gaps. With 500 µm and later 300 µm ring gaps, continuous tubes were obtained, slit and flattened into self-supporting tapes. After drying, foils



~350 µm thick were flexible and mechanically sound. Electrodes extruded with 300 µm slit die were calandered to 75 µm while retaining 30 % open porosity and good flexibility.

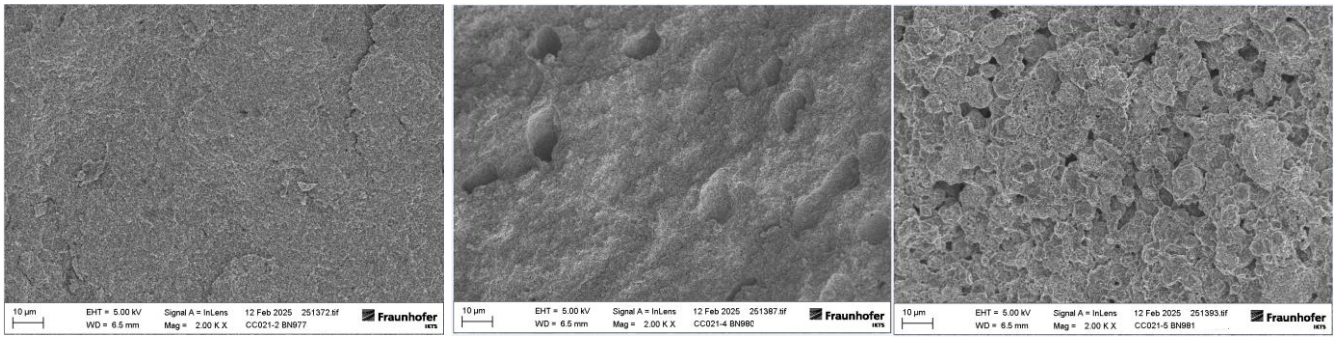


Figure 13 SEM images of extruded electrodes (left) (1) Life Power® P2, (middle) (2) Aleees A19, (right) (3) IBUvolt LFP200

For NMO, the same route was applied (NMO + Ensaco 250P + aqueous PAA), but mass rheology and downstream processing were significantly more challenging. Two formulations were tested. (1) with ~11.5 % PAA (dry) and higher moisture (~18 %) was machinable but strongly sticky, adhering to rolls and carrier films. (2) with 10 % PAA and lower moisture (~13 %) reduced sticking but became too stiff, causing high friction and unstable flow. Although NMO foils around 330 µm thickness and typical porosity could be produced, they were not sufficiently flexible, and calendaring was not successfully established. In coin-cell tests, the electrochemical properties (capacity and cycling stability) of the extruded LFP electrodes were determined. The cells were operated by utilizing Li metal anode foils to eliminate possible impacts from graphite electrodes. From the first charge for all LFP > 150 mAh/g capacity were found. Subsequent cycling showed capacity loss and degradation due to unclear cell failure. Electrodes after removing from the cells lost they lost their inner bond and fell apart. One possible explanation is the combination of binder decomposition due to pre-treatment during kneading of the mass and electrochemical processing. In contrast, extruded NMO electrodes fail electrochemically. Even the first charge

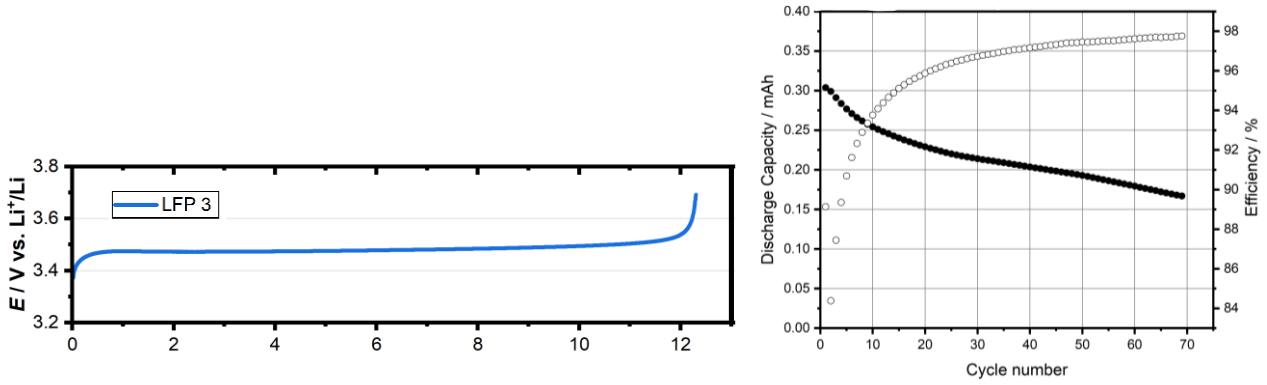


Figure 14 (left) Voltage of first charge LFP200 (IBUvolt), (right) cycling of the cell and degrading capacity and efficiency

4. Conclusions

Overall, LFP shows a mature, industrially viable process window from mass preparation through extrusion and calandering, while NMO still suffers from sub-optimal plasticity, die interaction and mechanical properties that prevent robust extrusion and post-densification. Further investigations into electrode stability are required to achieve stable performance.

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PERFORMANCE EVALUATION OF STRUCTURED POCS CATALYSTS FOR HYDROGEN PRODUCTION VIA AMMONIA DECOMPOSITION - (C116)

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Keywords: Ammonia cracking, hydrogen recovery, POCS

1. Introduction

NH_3 cracking is an emerging carbon-free route for distributed H_2 production [1], but is limited by thermodynamics, high heat demand, and the need for compact, high-throughput reactors. Conventional packed beds face limitations, including heat/mass transfer resistance, channeling, and pressure drops. Periodic Open Cellular Structures (POCS), instead, are a promising alternative [2] as their well-defined architecture offers uniform flow distribution, enhanced heat/mass transfer, low pressure drops, and high surface area. Thus, POCS are ideal for membrane assisted NH_3 cracking, where uniform flow, heat control, and low diffusion resistance are key for high conversion and efficient H_2 extraction [3]. This work assesses the intrinsic activity of Ru-K POCS as a baseline for membrane integration.

2. Materials and Methods

Two catalytic POCS units with a gyroid architecture, 70% porosity, and three-cell configuration were prepared from 3D-printed structures coated with 1 wt.% Ru and 3 wt.% K on Al_2O_3. Each cylinder measured 0.01 m in length and 0.027 m in diameter, with a 0.017 m central channel intended for a H_2-selective membrane and had a 0.15 g cm^{-3} catalyst loading. For testing, the POCS were placed in a reactor matching their external diameter, with the central channel filled by a metallic tube to replicate the presence of a membrane. The reactor was heated using an oven, and temperature was monitored with thermocouples. Catalyst was activated by exposing for 15 h to 75% H_2/N_2 450 °C. NH_3 decomposition was then tested at 425-450 °C, 2-6 bar, and 0.5-1.0 L_N/min, with steady-state conversions calculated from ten consecutive product measurements.

3. Results and Discussion

Figure 1, in which conversion is represented as a function of temperature for different weight hourly space velocities (WHSV) at 6 bar, indicates that ammonia conversion increased monotonically with temperature, which is consistent with the strongly endothermic nature of the reaction. The best performance were therefore obtained around 450 °C, where ammonia conversion was 43.9% when operating at a WHSV of 5522 ml/g/h, 45.6% when operating at WHSV of 4295 ml/g/h, and 53.3% when operating at WHSV of 3068 ml/g/h. Figure 1 also shows an inverse dependence of conversion on WHSV, which reflects the lower residence time at higher WHSV. While high conversion is desirable, high WHSV corresponds to larger throughput per catalyst mass, which is an important factor in reactor intensification. Therefore, an optimal balance between conversion and productivity is required when targeting system design.

The trend of ammonia conversion as a function of pressure for several space velocities and for the reactor operated at 450 °C is reported in Figure 2. As expected from the equilibrium shift associated with a reaction that increases total gas moles, decreasing reaction pressure significantly improved conversion. The highest performance was obtained at 2 bar, where ammonia conversion was 70.2% when operating at a WHSV of 3068 ml/g/h, 65.8% when operating at WHSV of 4295 ml/g/h, and 57.8% when operating at WHSV of 5522 ml/g/h. These results demonstrate that the standalone catalyst performance could be improved by reducing the operating pressure. However, while low-pressure operation favors conversion in standalone catalysts, the relevance of these results



must be reconsidered once hydrogen extraction through the membrane is introduced. Removing hydrogen from the reaction zone is expected to shift the equilibrium toward the products, potentially reducing the pressure-dependence penalty and enabling high conversion even at elevated pressures required by downstream applications.

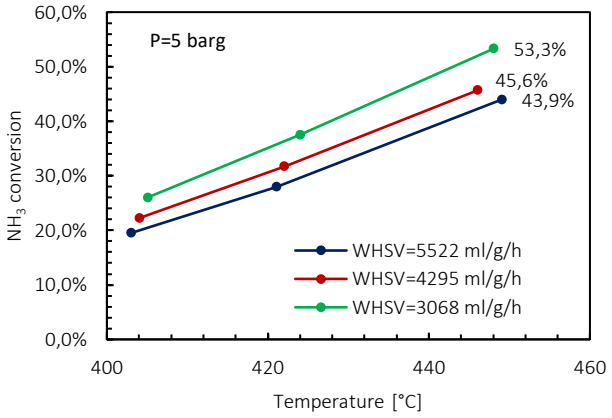


Figure 15: Effect of reaction temperature on ammonia conversion at different WHSV. The experimental results were obtained at an operating pressure of 6 bar.

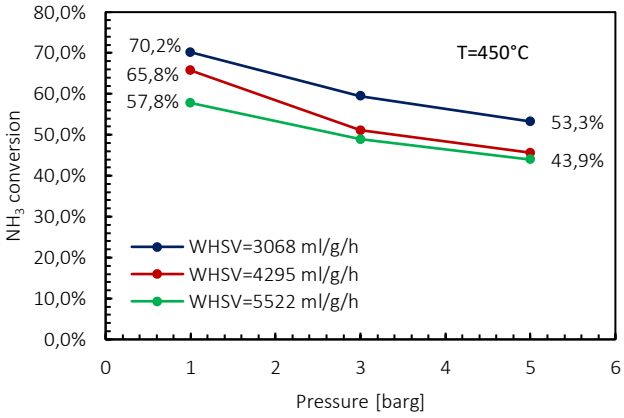


Figure 16: Effect of reaction pressure on ammonia conversion at different WHSV. The experimental results were obtained at an operating temperature of 450 °C.

4. Conclusions

Ru-K/Al_2O_3 POCS were tested for NH_3 decomposition, showing thermodynamically consistent behavior, with NH_3 conversion increasing with temperature, decreasing with pressure, and improving at lower WHSV due to longer residence times. A maximum conversion of 70.2% was reached at 450 °C, 2 bar, and lowest WHSV. These results establish the essential baseline required for evaluating the impact of H_2-permeable membranes. The next phase will investigate membrane-assisted operation.

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HUMAN-ROBOT COLLABORATIVE ASSEMBLY AND QUALITY ASSURANCE IN PROTON EXCHANGE MEMBRANE FUEL CELLS - (C120)

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Keywords: PEM fuel cells, robotic assembly, additive manufacturing, automated inspection, human-robot collaboration

1. Introduction

Scaling up polymer-electrolyte membrane fuel cell (PEMFC) production requires handling thin, fragile, and asymmetric layers repeatedly while maintaining tight tolerances and seal integrity. Within Italian national programmes on hydrogen technologies (funded by Italian National Electricity System Research programme PTR 2022–2024 and PTR 2025–2027"), a sustainable-by-design route has been designed coupling (i) a collaborative robotic cell for automated stacking and (ii) bipolar plates manufactured by additive manufacturing (AM). The present contribution consolidates those foundations and advances toward an inspection-enabled, human-centred workflow to improve placement accuracy, inline quality control, and explainability of the assembly process.

2. Materials and Methods

The assembly cell integrates a KUKA LBR iiwa 7 R800 with a customised OnRobot VGC10 vacuum end-effector and an Intel RealSense D435i RGB-D sensor [1]. A modular MATLAB-based GUI orchestrates perception and control while a CoppeliaSim digital twin mirrors off-line/on-line execution. For perception, we combine RGB-D pipelines with fine-tuned detection models and pose estimation; for Human-Robot Collaboration (HRC), we embed local speech-to-text (STT) with a task-aware dialogue manager and a Large Language Model (LLM-based) assistant [2]. Current efforts are focused on integrating inspection modules, including high-definition vision and 3D profilometry/laser for surface assessment, and thermo-vision for volumetric inspection of internal channels. Quality assessment closes the loop by detecting surface scratches, edge flaws, and channel occlusions before pressurisation steps.

3. Results and Discussion

Systematic tests on representative PEMFC parts demonstrated that foam-based area grippers induce buckling in thin layers. In contrast, the VGC10 achieves stable pick-and-place without permanent marks on the Membrane Electrode Assemblies (MEAs) or the gaskets, and supports pose correction via RGB-D sensing and compliant alignment. In parallel, bipolar plates were re-engineered for additive manufacturing by adopting horizontal builds and overhang-free channels, thereby reducing warping associated with residual stresses. These outcomes established the baseline for cost and cycle-time projections and guided the integration of quality checkpoints. The software stack (Fig. 1) comprises a twin-synchronised controller with logging of pose success rate, force-controlled alignment metrics, and speech-to-action latency. A multimodal cognitive layer, validated in a Meccano toy kit assembly scenario, combines local STT with a dialogue manager and an LLM assistant that explains task steps, checks sequence adherence, and accepts mixed-initiative commands; the same interaction capabilities run in the twin to de-risk behaviours before physical execution. This human-centred framework improves transparency, reduces operator cognitive load, and expedites what-if exploration of trajectories, tool changes, and inspection routines. Current work integrates inline inspection before and after placement. Vision and 3D profilometry target geometric/surface defects (scratches, chips, discontinuities at gasket interfaces), while thermal imaging probes



sub-surface anomalies or occlusions in internal channels. We intend to validate the thermographic inspection of complex additively manufactured plates using micro-computed tomography for ground truth on selected coupons. The goal is a closed-loop routine in which detected non-conformities trigger local rework or selective part replacement while keeping the stack-up within cycle-time budgets.

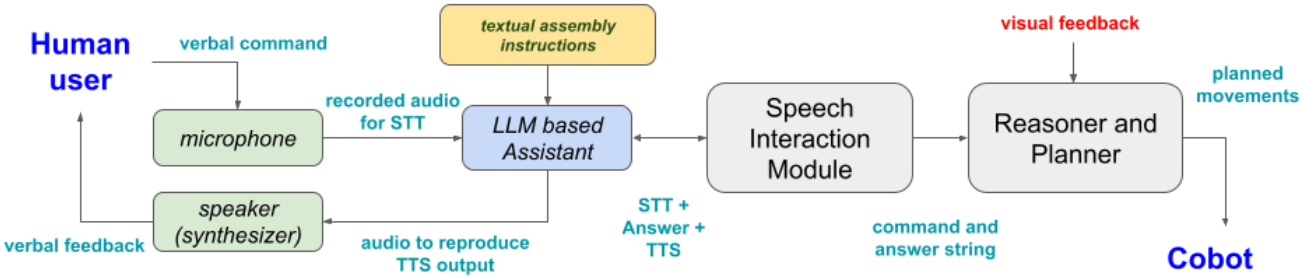


Figure 1. Main components of software architecture responsible for processing inputs, deciding and performing actions.

4. Conclusions

The proposed sustainable-by-design pathway couples collaborative robotic stacking, AM-oriented redesign of critical components, and a human-centred digital twin to improve accuracy, quality assurance, and operator experience in PEMFC manufacturing. Consolidated evidence on handling and AM lays the foundation for an inspection-enabled assembly loop now under integration.

Acknowledgements

This work was supported by the Italian National Electricity System Research programme, Theme 1.3: Three-Year Implementation Plan 2022–2024 "Integrated Hydrogen Technologies" (CUP B53C22008610001) and Three-Year Implementation Plan 2025–2027 (CUP B53C24009970001).

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SUSTAINABLE SYSTEMS: AN ADAPTIVE MANAGEMENT FRAMEWORK FOR PLANNING, PERFORMANCE, REPORTING AND STRATEGIC ORIENTATION - (C121)

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Keywords: Sustainable System, Smart Grids, Renewable Energy Communities, Sustainability Reporting

1. Introduction

This study conceptualizes a Sustainable System as a complex, adaptive and multi-actor socio-technical configuration embedded in Italian Inner Areas, which cover about 60% of the national territory and host nearly 25% of the population. These areas combine environmental and cultural heritage with socio-economic fragilities and governance weaknesses. Renewable Energy Communities (RECs) are framed as structural components of this system, integrating technology, local actors and collective objectives. While enabling sustainability transitions, RECs increase systemic complexity and uncertainty, requiring adaptive performance management and reporting systems capable of supporting long-term environmental, social and economic value creation.

2. Materials and Methods

The study adopts a conceptual framework integrating Sustainability Reporting (SR) characteristics, performance management framework under uncertainty [1], tactical urbanism as evolutionary planning logic [2], and smart grid infrastructures. SR is examined through stakeholder engagement, dynamic materiality assessment and Plan-Do-Check-Act (PDCA) processes [3]. The aim is to analyse how different frameworks, objectives, measures and feedback interact in complex and uncertain territorial contexts.

3. Results and Discussion

The analysis suggests that REC implementation, when not embedded within a systemic territorial governance perspective, does not automatically ensure coordinated and integrated sustainability outcomes. At the same time, SR, when applied in a rigid, compliance-oriented and KPI-driven manner, may produce certain limitations, including static indicators, short-term orientation and illusion of control [1]. Building on these concerns, Dynamic Public Governance (DPG) offers a complementary conceptual and operational response to these issues. By moving beyond fixed targets and hierarchical control logics, DPG promotes the integration of performance measurement with systemic dynamics, reduces risks of gaming and perverse incentives, and supports decision-making under conditions of uncertainty. Tactical urbanism, based on experimentation, incremental implementation and reversibility, reinforces this shift toward adaptive evolution rather than predefined outcomes [2]. Within this view, participatory stakeholder engagement and the co-construction of a dynamic materiality matrix become central elements for maintaining the strategic relevance of SR. Smart grids function as the enabling operational infrastructure of this model. By providing real-time, granular and transparent data on energy production, consumption and flexibility within RECs, they strengthen the dynamic dimension of SR. Although primarily related to the energy domain, these data enable more adaptive control mechanisms and horizontal coordination among actors, contributing to uncertainty management in complex territorial systems. Building on these perspectives, the study proposes an adaptive Management System interpreted as an integrated planning, performance and reporting mechanism. The Sustainable System is represented through a Causal Loop Diagram (Figure 1), mapping feedback loops and causal relationships across environmental, social, economic and governance dimensions.



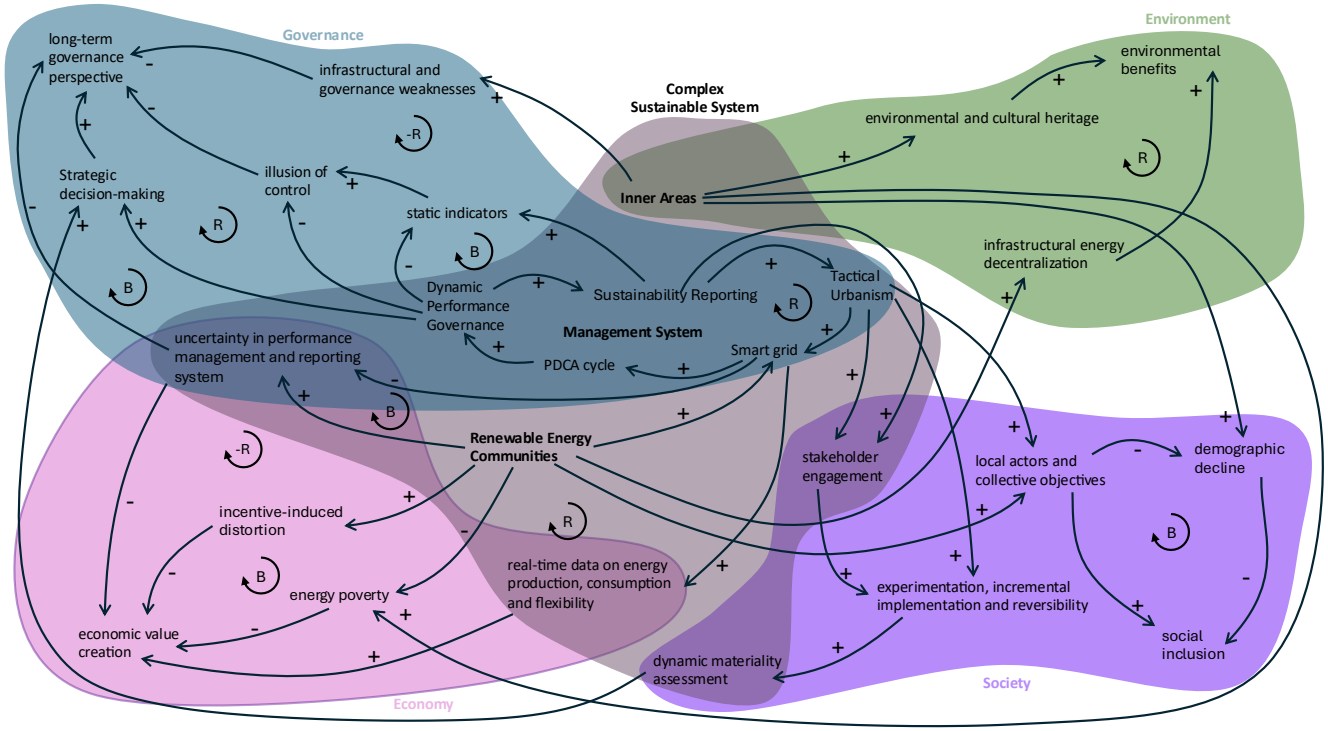


Figure 17. Causal Loop Diagram illustrating the complex interactions within territorial system

4. Conclusions

The Sustainable System identified in this study incorporates an adaptive Management System for planning, performance management, reporting and strategic orientation. Through the integration of SR with DPG framework, tactical urbanism and smart grids, the proposed model supports adaptive decision-making, participatory processes and long-term sustainable value creation under conditions of territorial and governance uncertainty, moving beyond static and compliance-oriented reporting approaches.

Acknowledgements

This work was supported by the Italian Ministry of University and Research (MUR) under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 4.1, DM 629/2024 – PhD programmes, co-funded by the European Union – NextGenerationEU (CUP: B74C24000420007).

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BIO-INSPIRED ELECTROCHEMICAL SYSTEMS FOR SUSTAINABLE HYDROGEN ACROSS THE VALUE CHAIN - (C122)

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Keywords: Hydrogen, Water, Bio-inspired systems, Catalysts, Electrochemistry.

1. Introduction

Hydrogen is a key energy vector supporting decarbonization across industry, transport, and energy storage, contributing to SDGs 6, 7, and 13. Water electrolysis enables renewable hydrogen production but faces limitations related to catalyst criticality, efficiency losses, and dependence on ultrapure water. As hydrogen demand increases, reliance on freshwater and scarce catalytic materials presents technological, environmental, and social challenges. Alternative water sources such as seawater, wastewater, and industrial effluents offer opportunities but introduce contaminants affecting system performance [1]. Additionally, Balance of Plant (BoP) components, including water purification and gas management, significantly influence overall efficiency and sustainability (reaching up to 60% CAPEX) [2]. Nature provides efficient and highly selective catalysts such as hydrogenases or formate dehydrogenases [3], offering inspiration for resilient electrochemical systems.

2. Materials and Methods

This work adopts a comparative approach, analysing conventional electrolysis and bio-inspired catalytic systems within the hydrogen value chain. It examines catalyst efficiency, water resource requirements, and system-level constraints, including BoP components. Enzymatic principles from enzymes (e.g. hydrogenases, formate dehydrogenases) are explored as models to achieve flexible electrochemical systems able of operating efficiently under realistic conditions. Experimental examples are discussed.

3. Results and Discussion

The sustainability of the hydrogen value chain depends not only on renewable electricity but also on resource-efficient production systems capable of operating with diverse water sources. Freshwater scarcity is a growing constraint, including from the social point of view, while alternative sources such as seawater, wastewater, and industrial effluents contain dissolved species including CO_2, ammonia, nitrogen compounds, hydrocarbons, etc. Conventional electrolysers require ultrapure water to avoid catalyst degradation, membrane fouling, and efficiency losses, limiting flexibility and increasing system cost. Biological catalysts such as hydrogenases enable highly selective hydrogen evolution, minimizing parasitic reactions and maintaining efficiency in chemically complex environment. Their catalytic sites combine optimized electronic structure, rapid proton transfer, and high stability with redox centres containing earth-abundant metals (Fe, Ni, S). Formate dehydrogenases reversibly catalyse CO_2 and formate interconversion [3]. Bio-inspired catalysts replicating these features may enable efficient hydrogen production with improved impurity tolerance and reduced reliance on critical materials. Nitrogen species illustrate both challenges and opportunities. Ammonia, common in wastewater and industrial streams, is both a pollutant and a promising hydrogen carrier due to its high hydrogen density and existing infrastructure. Electrochemical ammonia oxidation enables hydrogen recovery or conversion into nitrogen gas, supporting energy recovery and pollutant mitigation. Conversely, electrochemical nitrogen reduction enables ammonia synthesis from nitrogen using renewable electricity, providing a carbon-free hydrogen storage pathway. These interconnected reactions highlight adaptable electrochemical platforms capable of producing hydrogen, enabling ammonia-based storage, and supporting nitrogen and carbon



conversion, expanding the use of lower-quality water while integrating energy production, storage, and environmental remediation, strengthening the resilience, flexibility, and sustainability of the hydrogen value chain.

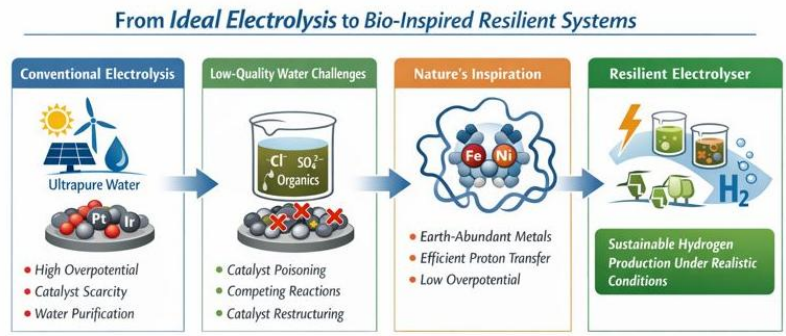


Figure. Bio-inspired electrochemical system enabling resilient and cost-effective hydrogen production using diverse water resources.

4. Conclusions

Bio-inspired electrochemical systems offer a transformative pathway toward resilient, cost-effective, and scalable hydrogen production. By enabling selective catalysis and operation with diverse water sources, these approaches can reduce dependence on critical materials and complex Balance of Plant infrastructure. Such adaptive platforms may lower system costs, improve operational robustness, and accelerate industrial deployment of sustainable hydrogen across integrated energy value chains.

Acknowledgements

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INNOVATIVE FUNCTIONAL GROUPS TO IMPROVE THERMAL DURABILITY AND PERFORMANCE OF ANION EXCHANGE MEMBRANES FOR GREEN HYDROGEN PRODUCTION - (C124)

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Keywords: Anion-exchange membrane, Anion-exchange membrane water electrolyser, H_2, Hydrogen production.

1. Introduction

Hydrogen production through anion exchange membrane water electrolysers (AEMWEs) is emerging as a promising route toward sustainable energy systems thanks to their use of low-cost materials and high operating efficiency. However, current anion exchange membranes suffer from limited chemical and thermal durability in harsh alkaline environments, primarily due to the degradation of quaternary ammonium groups. This work addresses these limitations by introducing novel pendant functional groups designed to enhance stability while preserving hydroxide conductivity, offering a new molecular-engineering strategy for next-generation AEMs.

2. Materials and Methods

Ionomers were synthesized via free-radical polymerization, and membranes were prepared by dip-coating commercial supports. Hydroxide conductivity was measured with a DC voltage scan in a four-electrode in-plane cell using a Scribner Membrane Test System 740 instrument. Ion-exchange capacity (IEC) of the membrane was determined by back-titration method. Structural and thermal properties were assessed by ^{1}H-NMR, FT-IR and TGA-IR. Membranes were tested in a MEA water electrolyzer setup.

3. Results and Discussion

This work explores a molecular-level design strategy based on pendant-group engineering to improve the stability of anion exchange ionomers. Instead of modifying the polymer backbone, different pendant group chemistries were introduced to tune the local environment around the cationic sites. By adjusting steric hindrance, electronic effects and hydration behavior, the goal was to reduce alkaline and oxidative degradation while preserving efficient ionic transport.

A series of polymers was synthesized via free-radical polymerization and characterized by NMR and IR spectroscopy. Thermal stability, evaluated by TGA, confirmed that the nature of the pendant cationic groups strongly affects the onset of functional-group degradation.

Thin supported membranes were prepared by dip-coating a commercial porous substrate, ensuring controlled morphology and mechanical reinforcement. Ion exchange capacity and hydroxide conductivity were evaluated, showing that increased chemical robustness did not compromise ionic conduction. In several cases, pendant-group modification also improved microstructural organization and hydration, supporting efficient hydroxide transport.

Durability was tested under alkaline and oxidative conditions representative of AEMWE operation. Comparative analysis revealed distinct degradation behaviors, confirming that pendant-group chemistry governs resistance to nucleophilic and oxidative attack.



These results demonstrate that tailoring the local chemical environment can suppress the dominant degradation pathways typical of quaternary ammonium groups.

The most stable membranes were integrated into membrane–electrode assemblies (MEAs) and tested under operating AEMWE conditions. Device-level measurements showed that molecular-level improvements translate into enhanced operational durability, validating the effectiveness of this design strategy beyond ex-situ characterization.

4. Conclusions

Pendant-group engineering improves ionomer stability, enhancing resistance to alkaline and oxidative degradation while preserving hydroxide transport. These materials are promising for AEM electrolysers, enabling cleaner green H_2 production. Future work includes scaling up synthesis, industrial membrane fabrication and membrane testing in stack configurations.

Acknowledgements

Research activities were conducted in partnership with Hyter, contributing resources and technical knowledge.

The project is funded under the National Recovery and Resilience Plan (PNRR) with the contribution of the European Union – NextGenerationEU, in compliance with Article 34 of Regulation (EU) 2021/241.

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WASTE DERIVED MOS_2 NANOSTRUCTURES FOR HIGH-PERFORMANCE SUPERCAPACITORS - (C125)

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Keywords: MoS_2, supercapacitors, industrial waste, coin cell.

1. Introduction

The energy transition requires efficient, low-cost, and sustainable energy storage, while industrial waste calls for circular solutions. Converting waste into functional nanomaterials reduces environmental impact [1][2]. Molybdenum disulphide (MoS_2) is promising for energy storage, but conventional synthesis is costly. This work develops a sustainable route to MoS_2 nanostructures from Mo-based waste, showing their effectiveness as supercapacitor electrodes.

2. Materials and Methods

MoS_2 was synthesized via a hydrothermal process from Mo-based industrial waste and thiourea. Morphology was analyzed by scanning electron microscopy (SEM) and Raman spectroscopy. Electrochemical performance was tested by cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) and electrochemical impedance spectroscopy (EIS) in a three-electrode set up, using graphene paper as substrate, or a coin cell configuration.

3. Results and Discussion

SEM analysis shows well defined MoS_2 nanostructures, like nanoflowers morphology (Figure 1 a) with lateral dimensions of a few nanometres. Raman spectroscopy also confirms the successful formation of MoS_2 by the presence of typical peaks (Figure 1 b), at 111, 144, 282, 334 and 374 cm^{-1}.

Electrochemical characterization was evaluated in a three-electrode cell configuration using 1 M ammonium sulphate ($(NH_4)_2SO_4$) as electrolyte. Cyclic voltammetry (CV) yields a specific capacitance of 272 F g^{-1} at 5 mV s^{-1} (Figure 2 a-b). CVs show a quasi-rectangular shape, indicative of a supercapacitor's behaviour. Galvanostatic charge-discharge (GCD) measurements provide a specific capacitance of approximately 300 F g^{-1} at 0.5 A g^{-1} with low IR drop, indicating efficient charge transport. Electrochemical impedance spectroscopy (EIS) was executed to study the interface electrode-electrolyte,

An Asymmetric MoS_2-based coin cell was assembled in ammonium sulphate electrolyte, using carbon black as counter electrode. This device delivers a specific capacitance of 106 F g^{-1} at 5 mV s^{-1} (CV) (Figure 2 c-d).



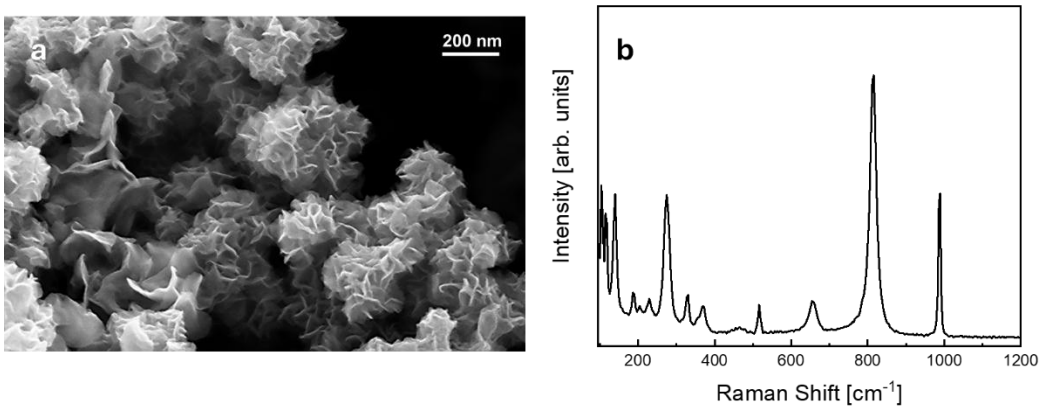


Figure 1. a) SEM image of the synthesized MoS_2 nanoflowers and b) Raman spectra that shows traditional MoS_2 peaks.

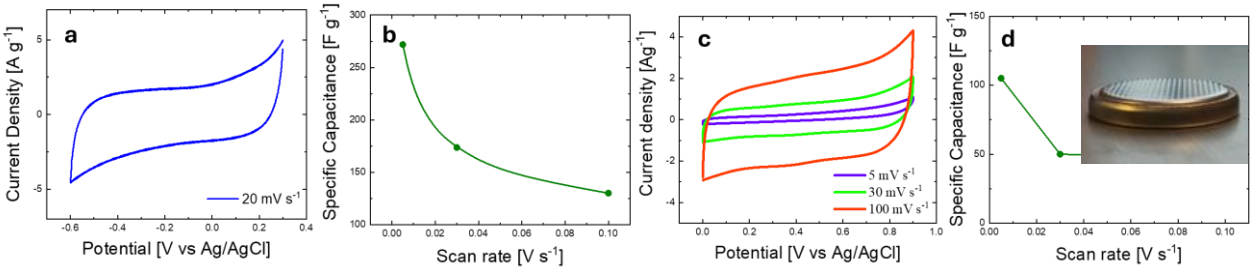


Figure 2. a) CV at 20 mV s^{-1} and b) specific capacitance of the MoS_2 in a three-electrode set-up; c) CV at different scan rate and d) specific capacitance in a coin cell configuration, the produced coin cell is shown in the inset.

4. Conclusions

This study demonstrates a sustainable and scalable route for converting Mo-based industrial waste into high-performance MoS_2 nanostructures through a simple hydrothermal process. The recycled material exhibits excellent electrochemical properties for supercapacitor applications, supporting its potential use in chemical energy storage. The proposed approach contributes to waste valorization, resource efficiency and the development of greener energy storage systems.

Acknowledgements

This research was funded by the Italian ministry MUR-PNRR project SAMOTHRACE (ECS00000022) by the European Union (NextGeneration EU).

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DUAL-FUNCTION MATERIALS FOR LOW-TEMPERATURE INTEGRATED CO_2 CAPTURE/METHANATION - (C126)

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Keywords: dual-function materials (DFM), integrated CO_2 capture and conversion (ICCU), CO_2 methanation.

1. Introduction

Integrated CO_2 capture and utilization (ICCU) is a promising transition route for mitigating flue-gas emissions while producing useful energy-carrying chemicals.[1] The process consists of repeated isothermal cycles of CO_2 adsorption and hydrogenation on a so-called dual-function material (DFM) placed in a flow fixed bed reactor. A typical DFM for methane production is Ni/Al_2O_3 (catalyst) combined with CaO (adsorbent), which however requires a high operating temperature (~600 °C) for adsorbent regeneration. Here, we report on DFMs using nickel or rhenium coupled to ceria (CeO_2) and/or a layered double oxide (LDO, *i.e.* Mg_2AlO_x), operating at moderate temperature (300 °C). These materials show good methane productivity and stability. Complementary investigations, including with advanced spectroscopies, reveal their unexpected behavior under cyclic operation.

2. Materials and Methods

A 12 wt% Ni-CeO_2 powder (120 m^2/g) was prepared from Schiff-base metal complexes.[2] Re-based materials consisted of either Re precursor directly impregnated and reduced (Re loading ~5 wt%) on five different oxide supports including commercial LDO (~200 m^2/g), γ-Al_2O_3 (157 m^2/g) and CeO_2 (123 m^2/g), or a mechanical mixture of the Re/γ-Al_2O_3 catalyst with LDO. Conventional CO_2 hydrogenation (CO_2:H_2:N_2=10:40:50%) and ICCU-methanation (7.5%CO_2/N_2, 33% H_2/N_2) were carried out at 300 °C in a fixed bed reactor equipped with a NDIR detector. The samples were characterized using a number of techniques including *operando* Raman/DRIFTS/XAS, NAP-XPS, STEM, SEM, and TPD/TPSR.

3. Results and Discussion

The Ni-CeO_2 nanomaterial, which is already a good methanation catalyst,[1] exhibits the highest ICCU performance, with up to 330 µmol of methane produced per gram of DFM per cycle of 8.5 min at 300 °C, and high stability over 50 cycles. Diluting Ni-CeO_2 in LDO generates up to four times more methane per mass of catalyst than Ni-CeO_2 alone, leading to a markedly reduced environmental footprint as measured by life cycle assessment.

Re-based DFMs (Fig. 1a) also show 100% selectivity to CH_4 whereas they are poor methanation catalysts in conventional CO_2+H_2 conditions (Fig. 1b).[3] Re/γ-Al_2O_3 catalyst mixing with LDO increases the methane productivity, and direct Re impregnation on LDO provides the best performance. However, the highest long-term stability and resistance to water impurities is shown by Re/CeO_2. *Operando* experiments on this DFM reveal that atomically dispersed Re species remain highly oxidized even under hydrogen (Raman); although carbonates are the most abundant surface species, formates and Re-carbonyls seem to play a key role (DRIFTS, Fig. 1c).



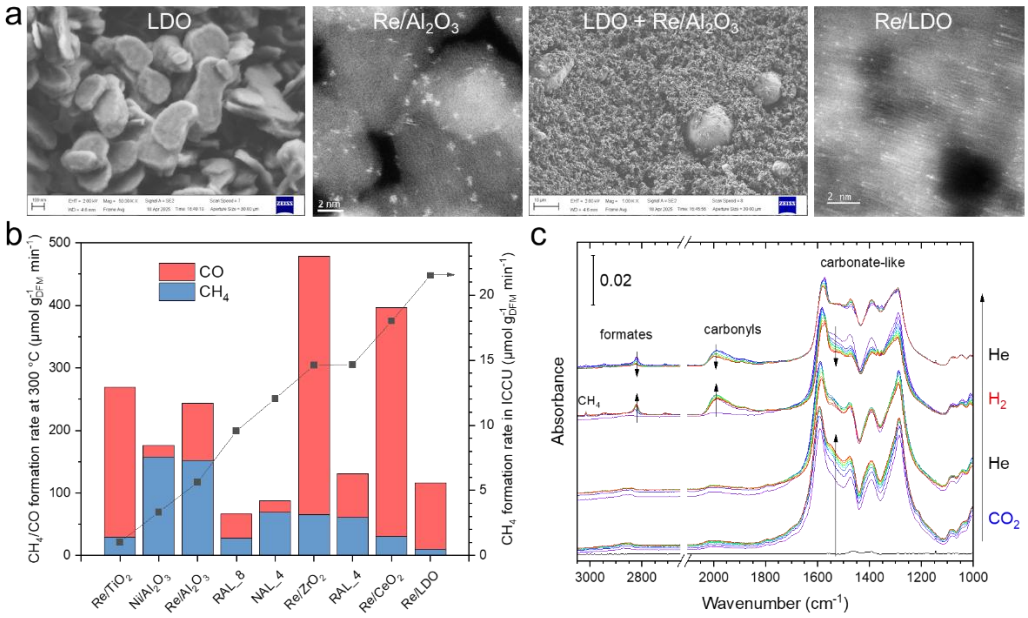


Figure 1. a) SEM and STEM images of LDO adsorbent, Re/γ-Al_2O_3 catalyst, LDO + Re/γ-Al_2O_3 mechanical mixture (RAL_*x*, where *x* is the dilution factor), and Re/LDO DFM. b) Activities in CO_2+H_2 reaction (bars) and ICCU-CH_4 (dots) at 300 °C. c) DRIFT spectra recorded throughout an ICCU cycle.[3]

4. Conclusions

Nickel or rhenium combined with ceria exhibits good performance in ICCU. Dilution in hydrotalcite-derived oxide increases the sustainability of the process. Notably, the search for efficient methanation DFMs should not be limited to methane-selective catalysts since the cyclic conditions applied in ICCU favor methanation.

Acknowledgements

This work was supported by the DuCaCO2 project, ANR-21-CE05-0023.

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POLYBENZIMIDAZOLES ARCHITECTURES FOR HIGH-TEMPERATURE PROTON-EXCHANGE MEMBRANES - (C127)

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Keywords: HT-PEM, polybenzimidazole (PBI), phosphoric acid doping, hyperbranched, proton conductivity.

1. Introduction

HT-PEMs extend PEM fuel cell operation to 80–180 °C with simplified water management; however, PFAS-based polymer membranes (e.g., Nafion) raise environmental concerns, and their performance is strongly influenced by hydration. Hydrocarbon-based polybenzimidazoles (PBIs) combine high thermal stability with imidazole sites that coordinate phosphoric acid, enabling efficient proton-transfer pathways.[1]

In this woek we develop linear–hyper-branched PBI architectures to achieve self-standing membranes with high PA uptake and improved retention.[2] Small additions of hyper branched-PBI (5-15 wt.%) to linear-PBI are explored to tailor phosphoric acid uptake, while retaining the high-temperature stability of the polymer backbone.

2. Materials and Methods

Linear polybenzimidazole (O-PBI) and hyperbranched polybenzimidazole (HB-PBI) were synthesized by mild polycondensation in Eaton's reagent. Membranes were prepared by solvent casting from 4 wt% polymer in DMAc and vacuum dried. Phosphoric acid doping was carried out by soaking in 85% H_3PO_4; selected samples were annealed at 150 °C under N_2 for 24 h. Thermal stability was evaluated by TGA/DSC, proton conductivity by in-plane measurements with MTS 740, and mechanical behavior by DMA temperature ramps in the viscoelastic regime.

3. Results and Discussion

Thermal characterization confirms that PBI architectures provide the robustness required for high-temperature PEM operation. TGA shows the main degradation step well above the targeted 80-180 °C window, while DSC reveals no detectable transitions up to 200 °C. Self-standing membranes were obtained by solvent casting for neat O-PBI (Membrane 1) and O-PBI/HB-PBI blends at 95:5 (Membrane 2) and 85:15 (Membrane 3). The central outcome is a clear, composition-driven increase in phosphoric acid uptake after doping (Figure 1).



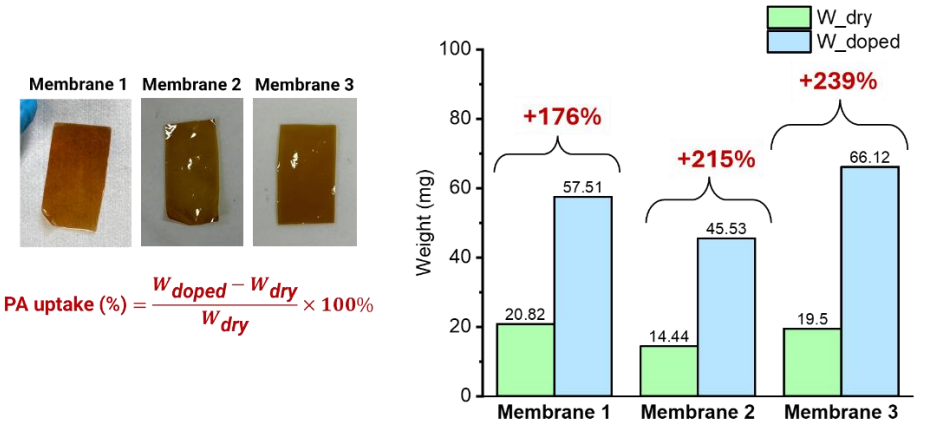


Figure 1- Photographs of the self-standing membranes, formula used for PA uptake calculation, membrane weight before and after doping in 85 wt.% H_3PO_4 at 70 °C for 16 h, and corresponding PA uptake (%).

This demonstrates that small HB-PBI additions provide an effective handle to modulate acid loading and, potentially, retention in an O-PBI matrix. In-plane conductivity of the PA-doped membranes was measured between 80 and 180 °C, and all the samples show a temperature-activated increase. Among the tested formulations, the 15 wt.% HB-PBI blend reaches ≈ 46 mS cm^{-1} at 180 °C and shows the more stable temperature dependence in the current measurements. Ongoing work is focused on confirming reproducibility and refining doping conditions.

4. Conclusions

Linear–hyperbranched PBI blend membranes were successfully developed as thermally stable, self-standing HT-PEMs. Small additions of HB-PBI significantly enhanced phosphoric acid uptake and improved proton conductivity, with the 85:15 blend emerging as the most promising composition.

The results demonstrate that controlled architectural modification represents a practical strategy to modulate acid loading and optimize proton transport in high-temperature fuel cell membranes. Ongoing work focuses on reproducibility, optimization of doping conditions, and long-term acid retention.

Acknowledgements

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INSIGHTS INTO THE RECONSTRUCTION OF MIXED OXIDES DURING ACIDIC OER - (C129)

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Keywords: OER, PEM water electrolysis, mixed oxides, electrocatalysis, surface reconstruction

1. Introduction

Renewable H_2 production using Proton Exchange Membrane Water Electrolysis (PEMWE) has emerged as a cornerstone for decarbonizing hard-to-electrify sectors due to its high efficiency, compact design, and rapid response to fluctuating renewable energy inputs. However, its large-scale deployment is hindered by the scarcity and high cost of Ir-based catalysts, which currently represent the benchmark for acidic OER owing to their good performance. In this context, there is a strong incentive to explore Ir-free or Ir-low content oxides capable of operating under acidic environments. Among them, transition-metal oxides have recently attracted attention since they can display remarkably high activity together with enhanced durability under strongly oxidizing conditions, due to their structural versatility and tunable electronic properties. Our work investigates mixed oxides containing Ir, Ru, or PGM-free materials. Most of them experience reconstruction during the OER that is dictated by their structural features and largely initiated by the loss of non-noble cations. Although these processes often lead to the formation of active site enriched surface layers, the resulting catalytic activity and stability remain highly sensitive to the parent lattice, especially to how the active sites octahedra or tetrahedra are interconnected. For instance, structures with face-sharing octahedra exhibit markedly higher resistance to dissolution and structural changes, whereas those with corner-sharing connectivity undergo more pronounced transformations.

2. Results and Discussion

Mixed oxides containing Ir, Ru, or Co show markedly different behaviors as oxygen evolution electrocatalysts depending on their crystallographic structure, cation distribution, active sites oxidation states, and metal–oxygen/metal–metal bonding environments. Across all systems, we find that catalyst reconstruction occurs either during operation or even upon simple immersion in acidic electrolyte.

Ru perovskites and pyrochlores display strong structure–activity relationships. Na doping in $Sr(Na)RuO_3$ significantly improves OER stability due to modifications on Ru oxidation state and an increment of RuO_6 symmetry, while R_2NiRuO_6 (R = Dy-Pr) pyrochlores shows that shorter Ru-O distances correlate with enhanced OER activity, with Dy_2NiRuO_6 remaining stable over 5000 CV cycles up to 1.7 V, which is a remarkable result for Ru catalysts. In R_2MnRuO_7, OER activity arises from a reconstructed $RuMnO_x$ surface, which forms under operating conditions. [1] PGM free mixed oxides based on Co are active and relatively durable to the OER in acidic media when stabilizing Co in tetrahedral sites, enabling surface reconstruction toward Co_3O_4 like layers.

For Ir mixed oxides, the connectivity of IrO_6 octahedra is identified as a key parameter of stability and activity. Face sharing IrO_6 networks, as found in hexagonal $AIrO_3$ (A = Sr, Ba), exhibit superior structural stability due to strong Ir-Ir and Ir-O interactions, whereas corner sharing frameworks undergo extensive surface reconstruction. We have studied the series of double perovskites Sr_2MIrO_6 (M = Ti, Fe, Sc, Y, Ni, Co, Mg, Zn, Ca cations) with corner sharing IrO_6 octahedra. Tuning the M site cation allows controlled adjustment of Ir oxidation state (4+ to 6+), Ir-O bond lengths, and octahedral distortion. Although reconstruction occurs across the series, the degree of stability contrasts with the activity trend, highlighting that performance depends not only on the reconstructed phase but also on the initial structural arrangement. The most active catalyst, Sr_2CaIrO_6, shows pronounced reconstruction even in electrolyte, forming a $IrOOH_x$ rich, hollow surface with very short Ir-Ir distances. Despite restructuring, Ir dissolution remains minimal due to the robust face sharing octahedral framework. Remarkably, very low Ir loadings (0.2 mg_{Ir} cm^{-2}) achieve PEMWE performance comparable to commercial catalysts containing ten times more Ir (Figure 1). [2,3] We are currently studying hexagonal Ir perovskites with face-sharing IrO_6 to compare their activity, durability and surface reconstruction with the corner-sharing Sr_2MIrO_6 perovskites.



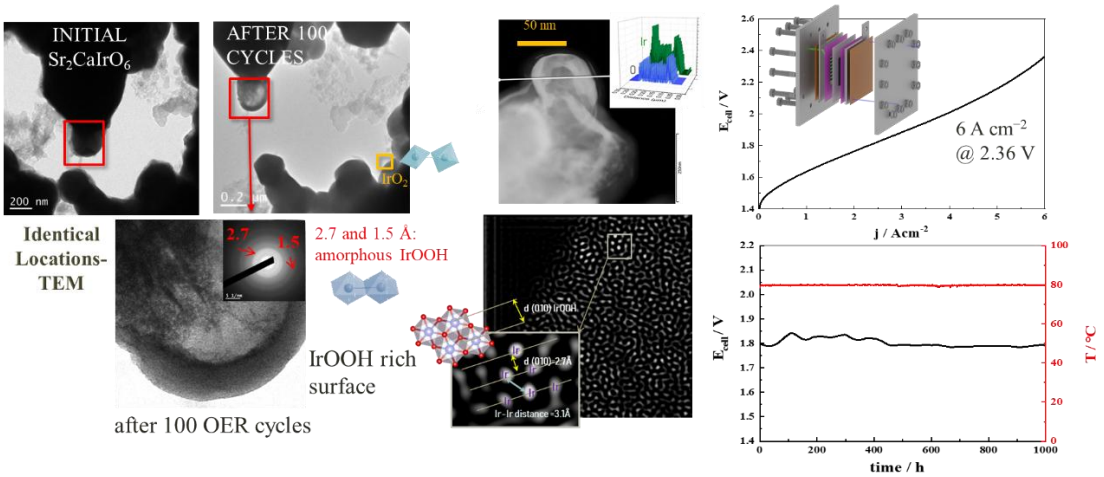


Figure 1: Surface reconstruction of Sr_2CaIrO_6 and PEMWE performance.

3. Conclusions

Mixed oxides undergo structural reconstruction during acidic OER. Ru and Co phases show activity trends linked to active sites-oxygen bond distances and surface reconstruction. In Ir catalysts, usually $IrOOH_x$ or IrOx surface layers are formed during reaction, however the final activity and durability strongly depend on the original crystal structure, particularly the connectivity of IrO_6 octahedra. Face sharing arrangements offer superior resistance to dissolution and restructuring, while corner sharing frameworks transform more extensively. Overall, establishing a clear correlation between OER performance and active sites connectivity is essential. Future work should further elucidate how octahedral or tetrahedral linking motifs govern reconstruction pathways, stability, and intrinsic catalytic activity, enabling the rational design of next generation oxide electrocatalysts for PEMWE.

Acknowledgements

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MODELLING OF A GAS TRANSMISSION NETWORK FOR HYDROGEN INJECTION: - (C130)

A Case Study of Sicily

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Keywords: Hydrogen Blending, Gas Network Digitalization, 3D Elevation Model, Mass Conservation.

1. Introduction

The need to decarbonize civil and industrial sectors positions hydrogen blending within existing natural gas networks as a key strategic solution, in line with European directives [1]. However, hydrogen injection significantly alters the fluid-dynamic properties of the mix. Standard macro-scale models lack the spatial granularity required to map specific nodal demands and accurately predict localized bottlenecks. This paper proposes a methodological framework constructing a 3D, high-resolution hydraulic model of the Sicilian transmission network (~2,000 km). It transforms geospatial open-data into a robust, georeferenced simulation model, capable of serving as a deterministic baseline for steady-state and dynamic simulations.

2. Materials and Methods

The framework vectorizes TSO cartography to build a network topology, advancing recent open-source network reconstruction efforts (e.g., SciGRID_gas) [2]. By integrating the Copernicus DEM, it assigns geodetic elevations to pipe, ensuring a 3D physical model. The consumption disaggregation allocates regional flows across georeferenced delivery nodes. Unlike regional top-down models [3], this approach enforces a strict mass balance between North African imports and final industrial, thermoelectric, and distribution consumptions.

3. Results and Discussion

The result is a fully balanced model of the Sicilian network, ready for hydrogen blending simulations. A quantitative extraction of the results demonstrates the framework's high fidelity. Firstly, the method accurately maps over 2,000 km of pipelines with diameters and attributes, and 171 hydraulic nodes with hourly injection or withdrawal values and altimetric elevations across the entire network. Secondly, the disaggregation operates using stringent mass balance equations, exactly equating the hourly flows reported by the National Dispatching Centre to the allocated consumptions for both single days and individual consumption categories.

By re-aggregating data, the model purified the spatial matrix (reducing 322 raw cabins to exactly 169 distinct municipal centers). Demographic ISTAT centroids were shifted and mathematically constrained to the most hydraulically coherent pipe sections, moving far beyond simple spatial proximity matching.

Regarding its impact, the generated model provides an accurate spatial resolution (Thermoelectric, Industrial, Civil) vastly superior to traditional macroscopic models, enabling accurate assessments of the network's hosting capacity for hydrogen mixtures. Furthermore, the methodology systematically processes peak-hour typical scenarios, allowing Transmission System Operators (TSOs) to effectively isolate sector-specific vulnerabilities. By identifying topological friction points under peak regional stress, the tool proves indispensable for planning localized capacity upgrades or strategic network retrofits ahead of large-scale green gas integration (Fig. 1).



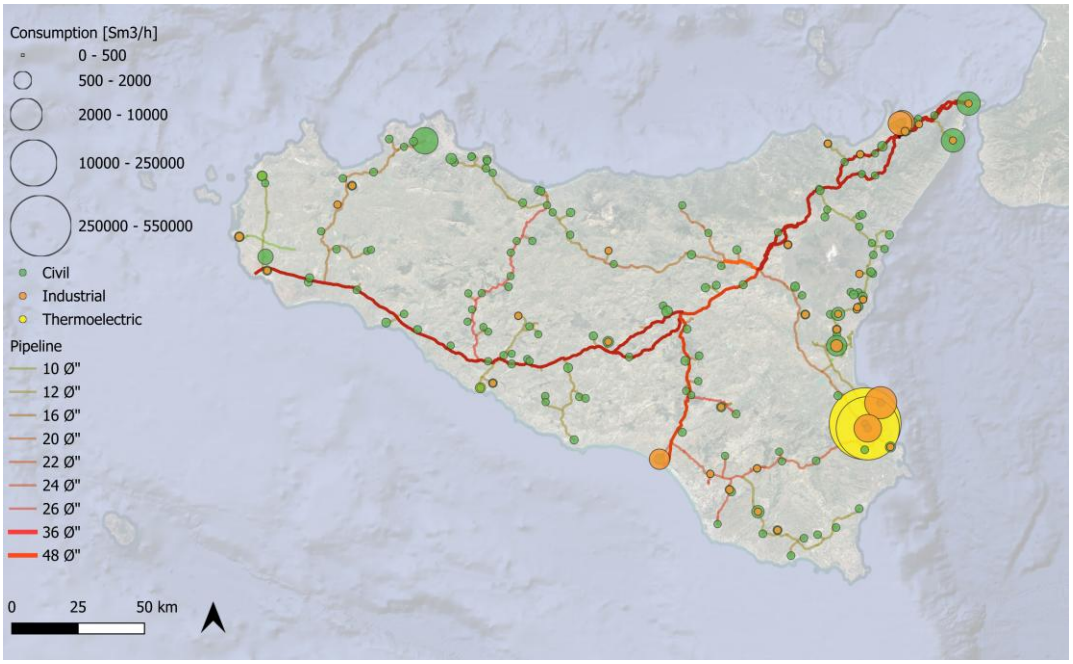


Figure 1. Spatial distribution of hourly gas loads disaggregated by sector (civil, industrial, thermoelectric) across the Sicilian pipeline network during the winter peak day (16/01/2024).

4. Conclusions

This study unifies national and regional gas network open data, providing a scalable framework for geospatial load disaggregation of gas consumption loads. The methodology guarantees 3D physical consistency, strict mass balance, and excellent sectorial load resolution. Future developments will include the integration of the primary compressor stations (Messina and Enna) to perform both dynamic and steady-state simulations of hydrogen injection under different operational scenarios.

Acknowledgements

This work was supported by CNR-ITAE.

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WHITE HYDROGEN IN THE ENERGY TRANSITION: TECHNICAL CHALLENGES AND RESEARCH FRONTIERS - (C131)

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Keywords: white hydrogen, white hydrogen value chain, hydrogen valleys, energy transition

1. Introduction

The transition toward climate neutrality requires scalable low-carbon hydrogen beyond electrolysis and CCS pathways. Naturally occurring "white" hydrogen has emerged as a potential complementary resource. While its origin, occurrence, and extraction technologies are increasingly examined, its role within broader hydrogen deployment frameworks remains insufficiently analysed. This work reviews technical challenges, techno-economic considerations, and integration perspectives, with particular attention to regional innovation dynamics, highlighting Southeast Europe and Bulgaria, as emerging research hubs.

2. Methods

A multidisciplinary qualitative assessment was conducted based on geological, geochemical, techno-economic, and engineering literature [1,2]. European and international pilot initiatives were reviewed to examine technological maturity, identify exploration and deployment constraints, and outline research priorities along the white hydrogen value chain.

3. Results and Discussion

Preliminary techno-economic assessments indicate that natural hydrogen extraction could achieve production costs of 1-2 €/kg, potentially below current green hydrogen benchmarks of 4-6 €/kg. However, economic potential alone does not ensure scalability, as commercialization is constrained by interconnected scientific, engineering, and systemic challenges across the value chain.

Exploration and localization remain fundamental uncertainties. Natural hydrogen systems are frequently diffuse, structurally controlled, and dynamically replenished, complicating resource quantification. Because hydrogen migration is governed by deep fault networks and fracture permeability, integrated geophysical methodologies are required.

Extraction presents material and operational constraints linked to hydrogen's physicochemical properties. Its low molecular weight and high diffusivity increase leakage probability and demand hydrogen-resistant casing materials, advanced sealing technologies, and continuous well integrity monitoring.

Processing requirements further influence feasibility. White hydrogen is commonly co-produced with methane, nitrogen, and carbon dioxide, necessitating optimized pressure swing adsorption or membrane-based separation systems to achieve ≥99.97% purity for fuel cell and industrial use.

Storage and transport constitute additional systemic barriers. Hydrogen's low volumetric energy density and potential for embrittlement of metallic infrastructure require adapted storage solutions, including salt caverns and depleted gas fields, alongside modular on-site compression and localized consumption models.



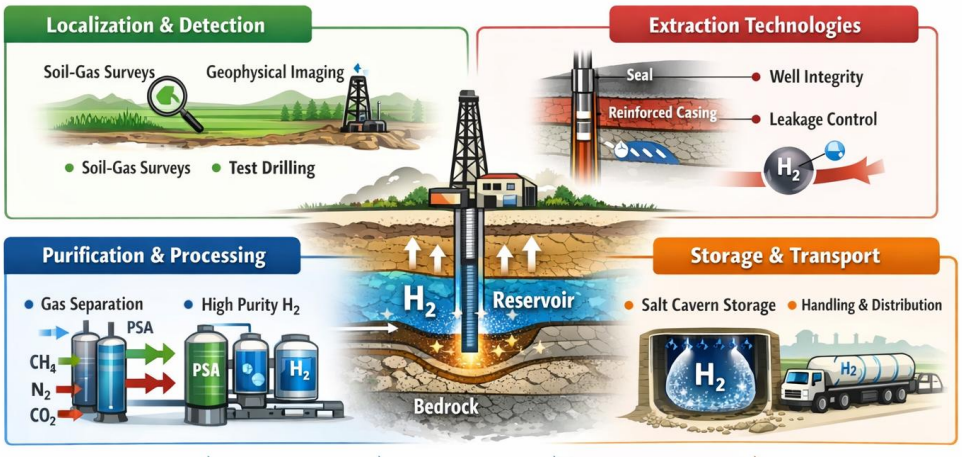


Figure: White hydrogen in the energy transition – technical challenges

Beyond technical constraints, regulatory uncertainty, environmental risk management, infrastructure gaps, and market integration dynamics shape deployment prospects. Regional hydrogen valleys may serve as controlled environments for hybrid architectures integrating geological and renewable hydrogen streams, thereby enhancing resilience and accelerating energy system transition.

4. Conclusions

White hydrogen represents a promising but technically immature frontier in the hydrogen economy. Key challenges include reliable detection, reservoir characterization, purification of mixed gases, and infrastructure adaptation. If responsibly developed within strong regulatory frameworks, it may complement green hydrogen and enhance energy security. Future research must prioritize pilot projects, reservoir monitoring, and hybrid integration into regional hydrogen systems.

Acknowledgements

European Union under the Horizon Europe program, Project No. 101136692, H2Start: Green Innovations in Hydrogen for a Sustainable Energy Transition. Bulgarian Ministry of Education and Science through the Bulgarian National Recovery and Resilience Plan, Project No. BG-RRP-2.004-0006-C02, Development of Research and Innovation at Trakia University in Service of Health and Sustainable Well-Being.

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RECYCLING PROCESSES FOR SOLID OXIDE ELECTROLYSIS CELLS - (C132)

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Keywords: Recycling wastes, Solid oxide cells, YSZ, Ionic conductivity, Phase separation.

1. Introduction

For better durability and cost, all the value chain of hydrogen technologies still needs improvements and R&I. The driving hydrogen development needs sustained research and innovation into breakthrough technologies for bringing new solutions to the market. H_2 production was mainly centered on conversion of fossil fuels and now on renewable energies via electrolysis process. Among different technologies, solid oxide electrolysis (SOE) shows high efficiency but suffers from short life time due to the high operating temperature. However, compared to Proton exchange membrane (PEM) electrolyzers, SOE cells are not using PFAS membrane and costly noble catalysts. But they are using several critical or strategical materials such as Ni or Y and La rare earth elements (REE) for the cell manufacturing, which must be recycled [1]. In this work, an innovative strategy for recycling and recovery of anode supported SOE ceramic components is presented.

2. Materials and Methods

Materials are commercials solid oxide cells (SOFC). Separation is done by mechanical scraping and chemical treatments. Solids are characterized by X-ray diffraction, scanning electron microscopy, thermal analysis and BET surface area measurement. Ion concentrations of the solutions were studied by Inductively Coupled Plasma Atomic Emission Spectrometry (ICP-AES). The conductivity level was measured by electrochemical impedance spectroscopy as a function of temperature.

3. Results and Discussion

After preliminary optimization of the leaching conditions of the raw materials entering its composition, i.e. selective separation of Ni^{2+} from other ions coming from the air electrode, and selective leaching of gadolinium-doped ceria GDC and yttrium-doped zirconia YSZ, the application of the complete process to the full commercial cell was successfully finalized. The entire optimized process is illustrated on Figure 1. It consisted in three successive leaching steps, leading to three leachates containing air electrode, nickel, and GDC precursors as nitrate ions, and YSZ as a final solid product.



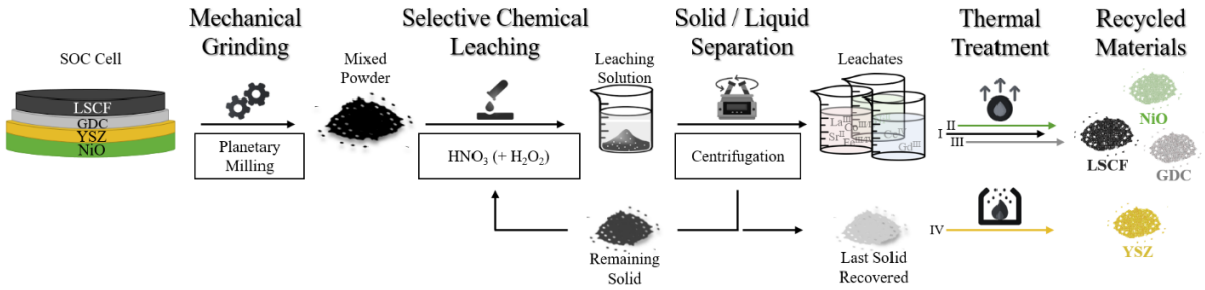


Figure 1. Scheme of the entire recycling process of a commercial solid oxide electrolysis cell [2].

Components including air electrode ($La_xSr_{1-x}Co_{1-y}Fe_yO_3$), nickel oxide (NiO), which accounts for about 50% of the cell weight, and yttria-stabilized zirconia (YSZ), which is coming from both the fuel electrode and the electrolyte, were successfully separated using Dissolution/separation steps. 90–92% of the total weight of initial Ni and YSZ can be collected. It was possible to recover the air electrode $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ (LSCF), NiO, GDC and YSZ powders at commercial purity grade.

The conductivity level of the recycled YSZ materials was measured in air by electrochemical impedance spectroscopy and is found comparable with commercial YSZ material, with a total value exceeding 6.4 10^{-3} S cm^{-1} at 700 ◦C. The contributions of grain and grain boundary conductivities to the total conductivity are clearly distinguishable at lower temperatures.

4. Conclusions

The use of a solution combining nitric acid and hydrogen peroxide, which are reagents used at industrial scale, is new and effective for separating the two electrolyte materials, YSZ and GDC, which are often found together in previous studies. The method focuses on the recovery of the four main materials that make up a commercial SOC, with the aim of reusing them in a new cell or in other applications, such as the NiO recovered with a purity of 99 %.

Acknowledgements

This work was supported by European Union's Horizon Europe research and innovation program under grant agreement N◦101058784.

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ARCHITECTED 3D-PRINTED FUEL CELLS AND NEXT-GENERATION CERAMIC ENERGY PLATFORMS - (C133)

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Keywords: Additive manufacturing, solid oxide electrochemical cell, reversible energy conversion.

1. Introduction

Solid oxide electrochemical cells enable highly efficient, reversible conversion between electricity and chemical fuels. Despite major advances in materials and cell chemistry, large-scale deployment remains constrained by planar and tubular stack designs composed of many discrete components. At the stack level, metallic interconnects and sealing elements dominate weight, volume, and failure modes, often accounting for more than three-quarters of the total system mass.

This architectural constraint limits compactness, gravimetric and volumetric power density, and durability, particularly under reversible and dynamic operation. Incremental improvements within two-dimensional designs have reached diminishing returns, shifting the scale-up challenge from materials to architecture.

Here, we introduce a fully three-dimensional, monolithic ceramic architecture enabled by additive manufacturing[1,2]. By adopting triply periodic minimal surface geometries, electrochemical functionality, gas distribution, and mechanical stability are integrated into a single self-supporting structure. Geometry and topology thus become active design variables, enabling lightweight, compact, and robust ceramic energy systems.

2. Materials and Methods

Monolithic three-dimensional ceramic fuel cell architectures based on triply periodic minimal surface gyroid geometries were fabricated by high-resolution digital light processing using 8 mol% yttria-stabilized zirconia slurries, followed by debinding and sintering to obtain dense, gas-tight monoliths with thin-walled electrolytes. Established NiO–YSZ and LSM–YSZ electrodes were applied to the internal gyroid surfaces by air-assisted wet coating and co-sintering, with platinum current collectors for testing.

Electrochemical performance was evaluated in fuel cell and electrolysis modes using impedance spectroscopy, current–voltage analysis, and galvanostatic stability tests. Structural and mechanical integrity were assessed by microscopy, X-ray micro-computed tomography, compression testing, and finite-element simulations to correlate architecture with thermo-mechanical behavior.

3. Results and Discussion

Transitioning from planar stacks to fully three-dimensional monolithic architectures produces performance gains unattainable through materials optimization alone (Fig. 1). Gyroid-based triply periodic minimal surface (TPMS) designs maximize space utilization by separating fuel and oxidant pathways within a continuous ceramic electrolyte, eliminating metallic interconnects and internal sealing components.

Additive manufacturing enables thin-walled gyroid electrolytes (~140–150 μm) with high density, ionic conductivity, and mechanical robustness arising from zero-mean-curvature geometry and stress redistribution by an external ceramic shell (Fig. 1). The resulting devices achieve specific power above 1 W g^{-1} and volumetric power density above 3 W cm^{-3}, nearly an order of magnitude higher than planar stacks, while electrolysis operation delivers mass- and volume-normalized hydrogen production approaching 10^{-3} Nm^3 h^{-1} g^{-1} and 10^{-3} Nm^3 h^{-1} cm^{-3} (Fig. 1).



These gains are achieved using established ceramic material systems and are accompanied by stable operation under steady-state, reversible cycling, and dynamic thermal conditions, confirming architecture as the dominant scale-up lever for next-generation ceramic energy platforms.

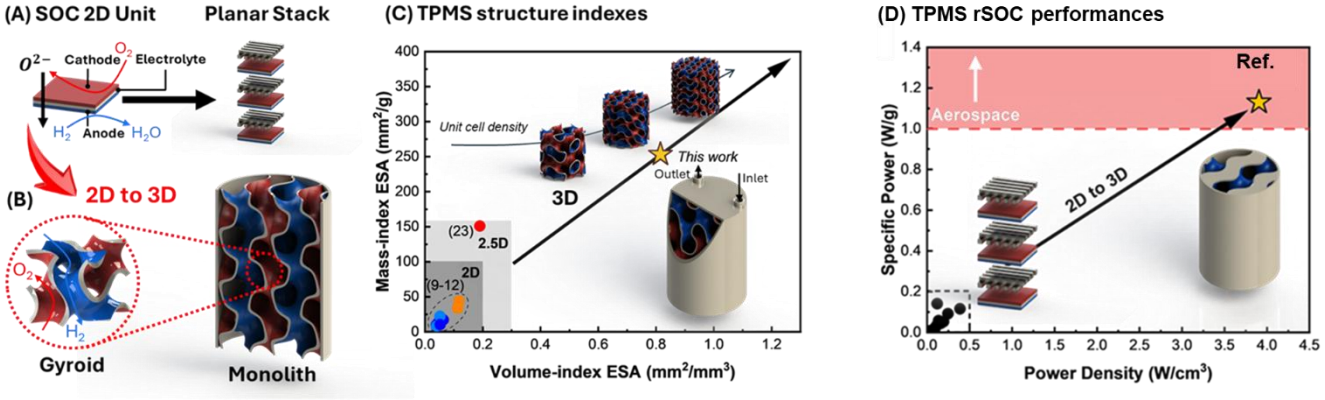


Fig. 1: Transition from planar to fully architected 3D ceramic fuel cells enabled by additive manufacturing, based on gyroid TPMS architectures. The monolithic design eliminates metallic interconnects and delivers order-of-magnitude gains in gravimetric and volumetric performance compared with state-of-the-art stacks.

4. Conclusions

This work demonstrates that fully architected, 3D-printed ceramic fuel cells enable a step change in gravimetric and volumetric performance by replacing planar stacking with monolithic architectures. By treating geometry as a functional design parameter, high performance, mechanical robustness, and reversible operation are achieved using established ceramic materials, opening pathways toward lightweight, compact, and scalable ceramic energy platforms..

Acknowledgements

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AMMONIA AS A H_2 CARRIER: ADVANCES IN NH_3 DECOMPOSITION TECHNOLOGIES AND INTEGRATION IN THE GREEN VALUE CHAIN - (C134)

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Keywords: Ammonia decomposition, Hydrogen production, Thermal catalysis, Electrocatalytic ammonia oxidation, Flow electrochemical cell.

1. Introduction

Ammonia is increasingly viewed as a strategic hydrogen carrier, and its efficient conversion to H_2 is a pivotal step in the green-ammonia value chain. Two approaches are particularly relevant and complementary: thermocatalytic NH_3 cracking, often intensified in hydrogen-selective membrane reactors, and electrochemical ammonia electrolysis. Thermocatalytic decomposition has been widely studied [1], yet it generally requires high temperatures (typically >550 °C). These conditions can complicate reactor design and catalyst stability, especially in the presence of water vapor. Moreover, in conventional packed-bed reactors (PBRs) the reaction is reversible and therefore constrained by equilibrium, with limitations becoming more severe at elevated pressure and at the high conversions targeted in compact, high-efficiency systems. Incorporating H_2-selective membranes, commonly Pd thin-film layers, addresses these constraints by continuously removing hydrogen from the reaction zone, shifting equilibrium and enhancing overall conversion and performance [2]. Electrochemical conversion, by contrast, is driven by an applied potential rather than thermal energy. In alkaline media, ammonia electrolysis can operate near ambient temperature: NH_3 is oxidized at the anode (ammonia oxidation reaction, AOR) while H_2 evolves at the cathode. Because AOR is thermodynamically less demanding than the oxygen evolution reaction, ammonia electrolysis can in principle achieve lower cell voltages than conventional water electrolysis.

2. Materials and Methods

An experimental setup based on a two-compartment flow electrochemical cell was employed, with the chambers separated by a commercially available anion-exchange membrane. Electrolytes with controlled concentrations were circulated through a two-chamber flow cell at moderate flow rates. The working electrode (WE) and reference electrode (RE) were positioned in the anodic chamber, while the counter electrode (CE) was placed in the cathodic chamber. Both compartments were operated under continuous-flow conditions. Electrocatalytic measurements Cyclic voltammetry (CV) and Chrono amperometry (CA) were carried out in a three-electrode configuration using a Pt-based catalysts and Pt-Ru catalyst. Gaseous and liquid products were periodically collected and analyzed by μGC and Ion chromatography.

3. Results and Discussion

Pt- and Ru-containing materials were evaluated as benchmark electrocatalysts because they can effectively bind and activate key intermediates formed during ammonia oxidation and decomposition. CV tests were performed in a potential range between 0 and 1 V_{RHE} showing a typical ammonia oxidation peak from 0.6 to 0.8 V_{RHE} [1]. CA tests were performed at -different potentials-showing higher current densities and higher hydrogen production for Pt-Ru electrode compared to Pt-based one.

More broadly, membrane enhanced thermocatalytic cracking and electrochemical ammonia conversion represent two distinct, yet potentially complementary, routes for producing hydrogen from NH_3. In this work, the two processes will be examined through a



critical, side-by-side comparison, highlighting their respective strengths, limitations, and practical trade-offs. The thermocatalytic route couples Ru-driven kinetics with H_2-selective membranes to intensify an equilibrium-limited, high-temperature reaction and deliver high-purity hydrogen. In contrast, the electrocatalytic pathway enables low-temperature, electrically driven conversion that can be directly integrated with renewable power sources; nevertheless, further advances are still required to improve catalyst durability and enhance cell-level efficiency.

4. Conclusions

These findings support Pt–Ru as a more effective benchmark for low-temperature, electrically driven NH_3 conversion, though durability and cell-level efficiency remain key targets for improvement. In parallel, the planned critical comparison with membrane-enhanced thermocatalytic cracking will clarify the performance trade-offs between high-purity, high-temperature equilibrium intensification and low-temperature electrochemical operation compatible with renewable electricity.

AcknowledgementsPart of this research was funded by CETPartnership, the Clean Energy Transition Partnership and the Swiss State Secretariat for Education, Research and Innovation (SERI) under the 2023 joint call for research proposals, co-funded by the European Commission (GA N°101069750) and with the funding organizations detailed on https://cetpartnership.eu/funding-agencies-and-call-modules. We gratefully acknowledge financial support from the Swiss Federal Office of Energy (SFOE) through the Grant No. SI/502842-01.

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HIGH-TEMPERATURE ENERGY STORAGE VIA REACTION CYCLES INVOLVING THE USE OF THERMO-CHEMICAL MATERIALS IN FLUIDIZED BEDS. - (C135)

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Keywords: Thermal Energy Storage, High Temperature, Fluidized Bed.

1. Introduction

High-temperature thermochemical energy storage systems (600–900°C) offer high energy storage density compared to sensible or phase-change technologies exceeding them by 10 and 5 times, respectively. They are among the few viable options for high-temperature applications and can rely on abundant, low-cost materials. Their integration with renewable energy sources and recovery of industrial waste heat support decarbonization pathways and contribute to long-term climate objectives, including PNIEC 2050 targets [1]. However, several technical barriers still limit their scale-up and market deployment. The aim is to investigate the cycling stability of the CaO-Mayenite/$CaCO_3$ thermochemical material (TCM) in a fluidized bed reactor in bubbling regime.

2. Materials and Methods

The TCM was synthesized via high-energy planetary ball milling of $CaCO_3$ and Al_2O_3, followed by sintering at 1000°C. The resulting powder was granulated (dp= 250 µm) using fluid bed spray granulation. Testing was conducted in a lab-scale Inconel fluidized bed reactor equipped with five thermocouples and mass flow controllers. After a zero-calcination step at 850°C to obtain pure CaO, 5 carbonation/calcination cycles were performed to evaluate stability, conversion and heat released.

3. Results and Discussion

The experiments were conducted at varying: superficial velocities, in terms of U/Umf ratio, total pressure and CO_2/N_2 concentration. Three tests were performed: B1 (15% CO_2, 5 bar, U/U_{mf} = 7.20), B2 (30% CO_2, 6 bar, U/U_{mf} = 3.43), and B8 (15% CO_2, 6 bar, U/U_{mf} = 2.80). Results obtained highlight the critical coupling between fluidization hydrodynamics and carbonation kinetics. To maintain a stable bubbling bed, the superficial gas velocity was kept at U/Umf > 2-3. This, combined with using Geldart Group B particles, ensured optimal gas-solid contact and prevented channeling. A key thermodynamic constraint is that the CO_2 partial pressure must exceed equilibrium ($pCO_2 \geq pCO_2$,eq). Analysis of tests B1, B2, and B8 showed that CO_2 concentration drives thermal performance: increasing pCO_2 accelerates kinetics and raises peak temperatures, with shorter reaction durations. Conversely, gas dilution reduces the driving force, leading to slower kinetics and a lower temperature lift (ΔT). As expected, the thermal evolution revealed two distinct zones: the dense and the lean zone. The dense zone is in the lower bed, where the thermocouple Tc6 (located 5 mm above the distributor) recorded a peak of about 800 °C. This area exhibits the most intense exothermic activity due to the high concentration of sorbent and fresh reactant gas. The lean zone, near the freeboard, reaches only 680°C due to lower solid concentration and volumetric heat generation. Cycling stability tests revealed a narrowing of temperature profiles over five cycles, signaling that the reaction completes faster due to sorbent sintering and reduced surface area. However, the perfect overlap of the final two (B10, B11) cycles confirms the material eventually reached a stable, quasi-steady state.



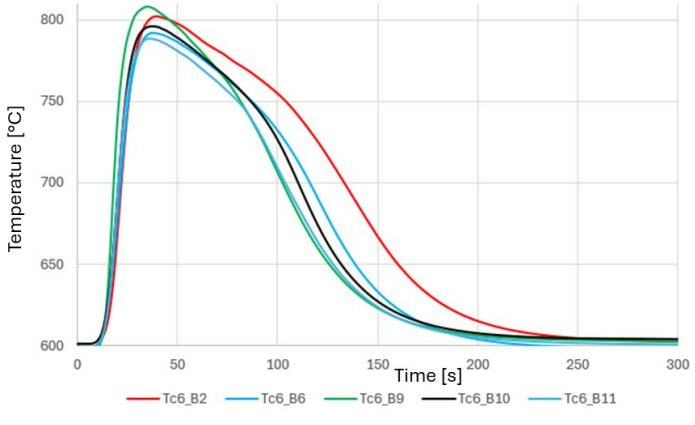


Figure 1. Cycling-stability behavior of the material through the temperature detected by the installed thermocouples during the discharging time in repeated B2 test conditions and calcination at 800°C in N2 atmosphere.

4. Conclusions

Based on TCM and bubbling fluidized bed reactor (FB-BB) test-rig results, this configuration is a promising, robust high-temperature energy storage technology. This work aimed to study long-term operational challenges by testing reactive pairs. These experimental investigations are essential to address criticalities and support the technology's scale-up, consolidating the reactor's performance for real-world renewable energy applications. To ensure economic and environmental sustainability, the system must use low-cost, non-strategic, and readily available materials.

Acknowledgements

This research was funded by MASE, the Italian Ministry of Environment and Energy Security, by means of the Research on Electric System fund—PTR 2025-27—Project 1.2: Electrochemical and thermal storage technologies, within Work Package 4—Thermal Storage: materials and innovative systems.

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HYDROGEN AND HIGH-ADDED VALUE PRODUCTION THROUGH AN INNOVATIVE BORATE-BOOSTED BIO-ALCOHOL UPGRADING - (C136)

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Keywords: Hydrogen, bio-alcohol, sodium metaborate, innovative process, carbon valorisation.

1. Introduction

Hydrogen is recognized as a key energy vector for reaching net-zero emissions by 2050. It acts as both an energy carrier and an important industrial feedstock. However, nearly 90% of the global hydrogen demand is still produced through fossil fuels, which results in substantial CO_2 emissions [1]. Therefore, finding alternative ways to produce hydrogen that cut down the carbon footprint while improving process efficiency and resource use is crucial.

A novel hydrogen production process has been developed and patented [2]. The process consists of a cyclic operation in batch reactors operating at mild temperature, with alternating additions of bio-alcohol and water to sodium metaborate. The process enables the simultaneous production of a hydrogen-rich gas and valuable carbon-based by-products, valorising the carbon fed with bio-alcohol.

2. Materials and Methods

A three-phase batch reactor vessel with a volume of 450 mL (Parr 4567) equipped with temperature, pressure and stirring control system (Parr 4848) was used for experimental tests. Bio-alcohol and water were alternatively fed to the reactor previously loaded with sodium metaborate. The reactor was heated up to the reaction temperature and the reaction was carried out for 6 h. The process produced solid, liquid, and gaseous products, that were off-line analyzed.

3. Results and Discussion

Using bioethanol, the process produced a hydrogen-rich stream with over 95% v/v at pressures between 30 and 45 bar. Under these conditions, the gas is suitable for blending into natural gas grids or using in fuel cells without extensive purification. Meanwhile, solid fraction mainly made up of oligoethylene chains with repeating $–CH_2–CH_2–$ units (average molecular weight ≈300 Da) has been produced, which has potential uses as synthetic lubricants and viscosity modifiers. The liquid phase contained valuable compounds, including 1-butanol, benzyl alcohol, and 1,1-diethoxyethane. The combination of the analyses of the different products allowed us to close the material balances for the process (up to step 4). Figure 1 shows the Sankey diagram for the overall material balance. Under current conditions, approximately 30% of the ethanol fed is converted. As shown in Figure 1, approximately 10% of this is converted to gas, while the remainder is converted primarily to high-value oxygenated organic compounds.



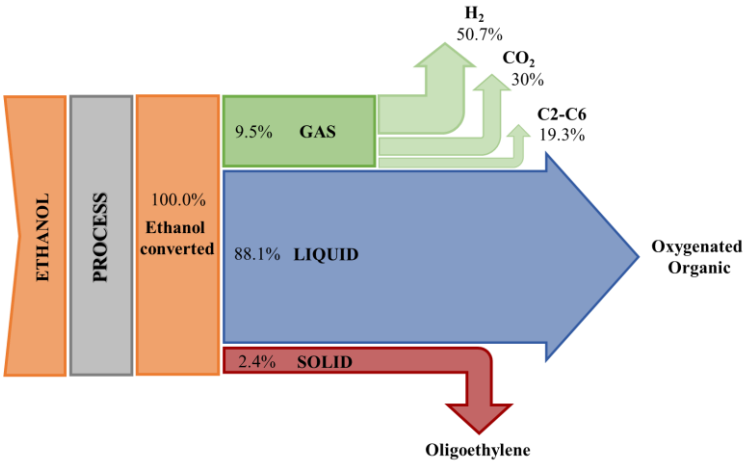


Figure 1. Sankey diagram for the process mass balance (four steps).

When we used crude glycerol, hydrogen selectivity reached about 55% v/v, producing a gas stream that works well with downstream upgrading processes like methanation to synthetic natural gas. The hydrogen generated in this process also enabled further transformations into valuable chemicals such as 1,2-propanediol and thermally stable aromatic resins in the solid phase. These findings show that the process can adapt to various bio-based feedstocks and adjust product distribution based on substrate structure.

4. Conclusions

Sodium metaborate proved to act as a reaction promoter, easing one-pot bio-alcohol dehydrogenation and carbon-carbon coupling reactions. Merging hydrogen production with carbon upgrading in a single reactive platform marks a major step forward in sustainable hydrogen technologies. By linking high-purity hydrogen generation with creating marketable by-products from inherently CO_2-neutral bio-alcohols, this process offers a promising pathway for next-generation low-carbon hydrogen systems. Future research will address the improvement of the overall conversion of bio-alcohol in order to improve the yield to both hydrogen and high-added value products.

Acknowledgements

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MEDIUM-TEMPERATURE ENERGY STORAGE SYSTEMS USING CONCRETE AND PHASE CHANGE MATERIALS. - (C137)

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Keywords: TES, SHTES, SHTES, CSLHTES, ETES

1. Introduction

Medium-temperature Thermal Energy Storage (TES) systems, up to 400°C, are essential for the use of both waste heat from industrial processes and for heat produced by renewable sources (solar energy). ENEA has been developing these medium-temperature thermal energy storage systems for years. After having developed systems based on sensible heat (Sensible Heat Thermal Energy Storage – SHTES) and system based on latent heat (Latent Heat Thermal Energy Storage - LHTES), ENEA is currently engaged in the study and development of combined sensible/latent heat systems (Combined Sensible-Latent Thermal Energy Storage - CSLHTES). In addition to thermal energy storage-only systems, ENEA is also committed to the development of thermal conversion and storage systems (Electro-Thermal Energy Storage - ETES), particularly using cement-based materials.

2. Combined Sensible-Latent Thermal Energy Storage

The sensible heat storage systems developed in ENEA use cement-based materials as the storage medium. In collaboration with the University of Perugia, new concretes were developed and characterized with the addition of shape-stabilized phase change materials ($NaNO_3$-KNO_3 – 60%-40%wt – solar salt), capable of withstanding temperatures up to 400°C. These materials were then used to build laboratory-scale modules, which were subsequently characterized in the temperature range between 200°C and 300°C. Latent heat thermal storage systems developed in ENEA always use solar salt as the phase change medium. Over the years, heat exchange phenomena during the melting and solidification phase of PCM, crucial for energy storage performance, have been studied, and this has led to the creation and characterization of LHTES modules, always at laboratory scale. Thermal storage systems that combine the use of both systems are currently being studied. Specifically, a SHTES module and a LHTES module have been connected in series. The thermal characterization phase of this CSLHTES system is underway using the SOLTECA3 facility at the Casaccia research center (figure 1). Also, a machine learning analysis is being conducted.

3. Electro-Thermal Energy Storage

The electro-thermal conversion and thermal storage systems being developed in ENEA are based on the coupling of a direct electro-thermal conversion system by Joule effect and a sensible heat thermal storage system, which uses a cement-based material as the storage medium. Initially, a laboratory-scale module was developed and characterized, using the ATES facility at the Casaccia research center (figure 2), in which, during the charging phase, the Joule effect occurs inside the metal tube. The heat thus generated is then transferred, by conduction, to the storage medium. In the subsequent discharging phase, a heat transfer fluid is circulated inside the same tube. A new ETES system is currently being studied, in collaboration with the University of Perugia, in which heat generation via the Joule effect occurs directly inside the cement-based storage medium. To do this, a new cement-based material with dissipative (conductive/resistive) properties has been studied and developed.





Figure 1. SOLTECA3 facility with CSLHTES module.



Figure 2. ATES facility with ETES module.

4. Conclusions

This work provides an overview of medium-temperature storage system developed and under development in ENEA. In particular, the development of a CSLHTES module consisting of two modules, a SHTES and a LHTES connected in series, is illustrated. Subsequently, the development of a new ETES system was illustrated, with heat generated via the Joule effect, which uses a cement-based material as storage medium. A cement-based material with dissipative (conductive/resistive) properties was also developed as the storage medium for this system.

Acknowledgements

This research was funded by MASE, the Italian Ministry of Environment and Energy Security, by means of the Research on Electric System fund—PTR 2025-27—Project 1.2: Electrochemical and thermal storage technologies, within Work Package 4—Thermal Storage: materials and innovative systems.

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THE ROLE OF ELECTRICITY STORAGE IN THE FUTURE ITALIAN ENERGY SCENARIOS - (C138)

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Keywords: Flexibility, Batteries, vRES, Adequacy

1. Introduction

Recent European energy policies focused on decarbonization aim to significantly increase the electrification of the energy systems. This shift is strongly connected to the decarbonization of electricity production and consumption processes and, thus, to the renewable energy penetration. The increasing share of variable renewable energy in the power system introduces a range of operational challenges, clearly reflected in the changing shape, variability, and uncertainty of the net load. These developments pose critical implications for system security: dispatchable units must cycle more rapidly and frequently, as they are essential providers of system services and short-term operational flexibility, including stability on sub-second timescales. Electrical storages are commonly identified as a means that can support in increasing the flexibility in the power grids, thus allowing for a higher share of intermittent renewable energy sources.

2. Materials and Methods

The analysis combines two complementary modelling approaches. First, a TIMES-Italy model represents the entire national energy system across all sectors and is used to develop alternative long-term energy transition scenarios. For each scenario, a Unit Commitment and Economic Dispatch (UCED) model of the Italian electricity system – based on the SAInt software - is implemented to capture short-term operational dynamics. This model enables an in-depth assessment of system implications in terms of unit commitment and dispatch patterns, short-term operational requirements, reliability indicators, renewable curtailment, market prices, and transmission line congestion.

3. Results and Discussion

The integrated TIMES–SAInt assessment shows that alternative decarbonisation pathways, characterised by different levels of variable renewable energy sources (vRES) penetration, fundamentally reshape the hourly residual demand profile. This reconfiguration of net load dynamics generates markedly different flexibility requirements for the Italian power system by 2050, with significant implications for Energy Not Served (ENS) and renewable curtailment rates across technologies and market zones.

Across all scenarios, increasing vRES penetration amplifies both intra-day and seasonal variability. Daily flexibility needs are primarily driven by solar diurnal cycles, whereas monthly variability reflects seasonal wind patterns and demand fluctuations.

Battery Energy Storage Systems (BESS) consistently mitigate short-term variability, substantially reducing curtailment and contributing to daily balancing. In high-vRES configurations, BESS discharge increases proportionally with renewable penetration; however, their contribution to system adequacy remains limited. Even under extensive storage deployment, the system requires at least 30 GW of efficient dispatchable capacity to meet adequacy standards. This confirms that BESS mainly address hourly flexibility, whereas seasonal balancing depends on firm low-carbon resources such as nuclear or carbon capture and storage (CCS).



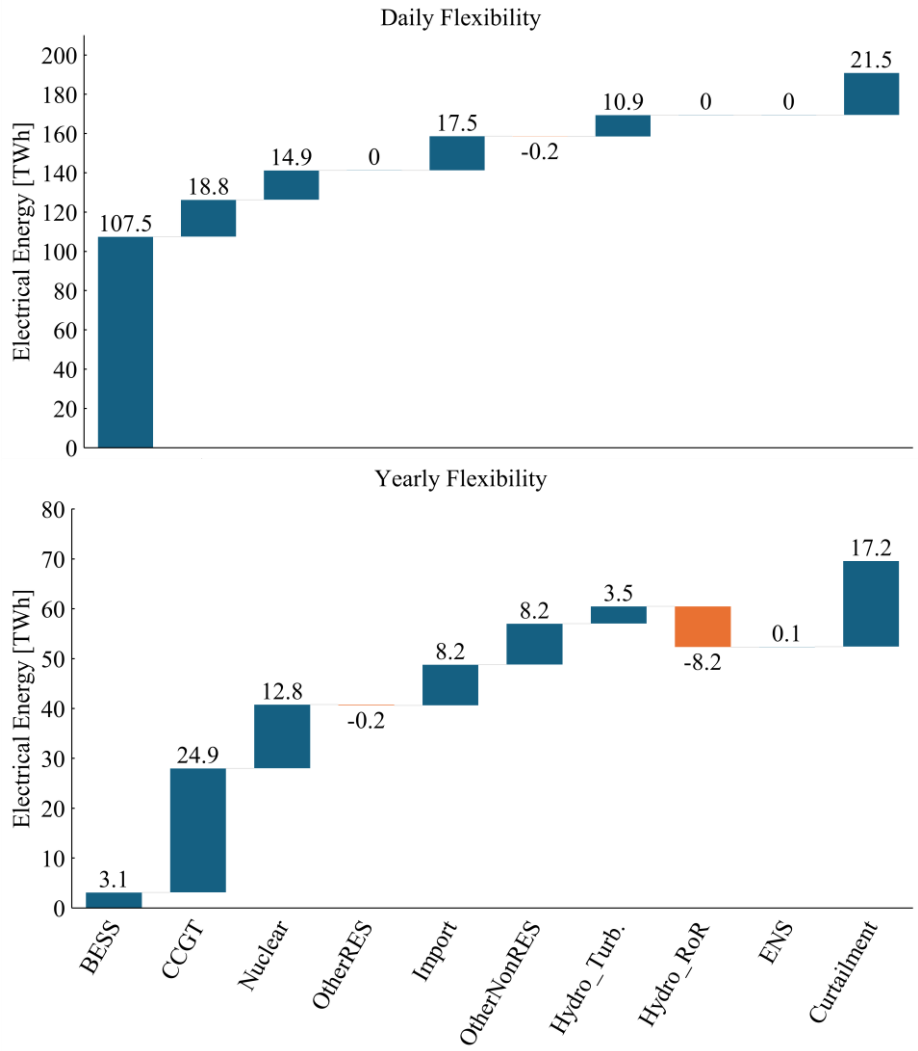


Figure 18: Role of BESS in Meeting Flexibility Requirements

System-wide impacts vary significantly across scenarios. Configurations lacking dispatchable low-carbon technologies exhibit substantial ENS, while scenarios integrating nuclear or CCS show markedly lower ENS and reduced marginal abatement costs. Price dynamics also diverge across pathways: higher vRES shares compress arbitrage spreads, thereby reducing BESS profitability despite increased operational intensity.

Overall, the results highlight that BESS are indispensable for short-term flexibility provision and curtailment reduction, yet insufficient to guarantee seasonal adequacy. A balanced portfolio combining storage, flexible thermal capacity, interconnections, and firm low-carbon generation remains essential for a resilient net-zero power system.

Finally, the integrated modelling framework provides a detailed operational validation of the long-term capacity expansion pathways generated by the TIMES model. The higher temporal and technical resolution of the UCED model enables a refined assessment of operational feasibility, reliability, and market outcomes, fully accounting for the key technical characteristics of the power system.

4. Conclusions

The integrated TIMES–UCED framework highlights the central role of system flexibility in achieving reliable and cost-effective decarbonisation of the Italian power system. Rising vRES penetration increases residual load variability, ENS and curtailment,



especially in the absence of firm dispatchable capacity. While BESS effectively mitigate short-term variability and reduce curtailment, they cannot ensure seasonal adequacy. Higher vRES shares also compress price spreads, limiting storage profitability. Overall, a diversified flexibility portfolio combining storage and firm low-carbon resources is essential.

Acknowledgements

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CONTROLLED THERMAL OXIDATION OF $Ti_3Al(1-X)TmxC_2$ (TM = Sn, Si) MAX PHASES FOR THE DEVELOPMENT OF NANOSTRUCTURED LI/NA-ION BATTERY ANODES - (C140)

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Keywords: Battery, MAXphase, Electrode, Anode, Nanostructurization.

1. Introduction

The growing demand for sustainable and cost-effective energy storage systems is driving the search for advanced anode materials for both lithium- and sodium-ion batteries. While graphite dominates Li-ion technology, it suffers from safety concerns at high current rates and is unsuitable for Na-ion systems. Conversion/alloying oxides offer higher capacities but undergo severe volume changes, leading to low cycling stability.

MAX phases have emerged as promising precursors for negative electrode materials due to their layered structure, chemical tunability and electronic conductivity. The electrochemical behavior of the pristine and partially oxidated MAX phases $Ti_3Al_{(1-x)}Tm_xC_2$ (Tm = Sn, Si) has been studied to evaluate the reaction mechanisms and performances in Li- and Na-ion batteries.

2. Materials and Methods

$Ti_3Al_{(1-x)}Tm_xC_2$ (Tm = Sn, Si) MAX Phases were prepared with SPS (Spark Plasma Sintering) and thermally treated under controlled atmosphere to induce partial oxidation and formation of active oxide phases on the surface of the material particles. Structural and morphological characterization was performed by in-situ (XRD) X-Ray Diffraction and electron microscopy. Electrodes were prepared using a conventional slurry-casting method and tested in Li-ion and Na-ion cells.

3. Results and Discussion

In situ XRD and Scanning Electron Microscopy (SEM) revealed that the thermal oxidation of Sn- and Si-containing MAX phases starts at ~500–700°C, with the progressive production of a nanocomposite architecture consisting of a conductive MAX Phase core decorated by transition metal oxide nanoparticles (10–20 nm). At higher temperatures the material decomposition is promoted. By controlling the treatment, a fraction of MAX phase can be so preserved, ensuring electronic conductivity and mechanical integrity of the oxidized material.

Electrochemical tests in Li half-cells demonstrate that oxidized Sn-rich samples deliver significantly higher reversible capacities than pristine MAX phases, confirming that charge storage is governed by the oxide fraction. The first cycle involves SnO_2 conversion ($SnO_2 + 4Li^+ + 4e^- \rightarrow Sn + 2Li_2O$) followed by reversible alloying/dealloying ($Sn + xLi^+ + xe^- \rightleftarrows Li_xSn$). Although the initial Coulombic efficiency is limited by partial irreversibility and SEI formation, it rapidly stabilizes above 99%. The conductive MAX core buffers volume changes and suppresses pulverization, enabling stable cycling over hundreds of cycles. For the best material tested, capacity values is approximately 300 mAh g^{-1} at C/10, with a satisfying capacity retention at different current values



(Figure 1). In Na half-cells, similar mechanisms occur, with lower capacity values due to the larger ionic radius and reduced Na–Sn reactivity [1].

Preliminary studies show how Si-rich samples exhibit comparable electrochemical performances with the Sn-based systems in Li-ion half-cells. The electrochemical reaction occurring at the electrode interphase are similar to the ones of the Sn-based materials, even if the overall reactivity of the oxidized $Ti_3Al_{(1-x)}Si_xC_2$ MAX Phase is lower, considering the higher theoretical specific capacity of the material.

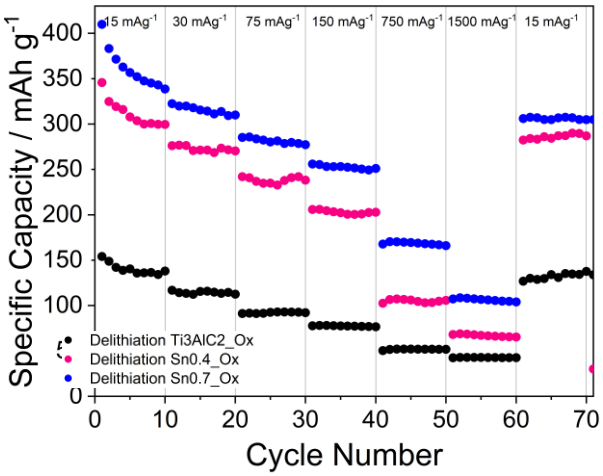


Figure 1

Figure 1. Electrochemical behavior of different oxidized $Ti_3Al_{(1-x)}Sn_xC_2$ MAX phases at different current values.

4. Conclusions

Oxidized $Ti_3Al_{(1-x)}Tm_xC_2$ (Tm = Sn, Si) MAX phase represents a promising dual-purpose anode material for lithium- and sodium-ion batteries. The combination of conductive layered domains and active oxide phases enables stable cycling, good rate capability and enhanced structural robustness. This approach provides a viable strategy for designing multifunctional MAX Phase-derived electrodes for next-generation energy storage technologies.

Acknowledgements

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COUPLED ATES–DHN SIMULATIONS: ASSESSING THE IMPACT OF HYDROGEOLOGICAL, THERMAL AND ENERGY PARAMETERS ON INTEGRATED SYSTEM PERFORMANCE - (C143)

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Keywords: Thermal energy, Storage, Coupled numerical simulations, District heating, Aquifers.

1. Introduction

The main challenge in developing renewable-based heating and cooling plants is addressing the intermittent availability of renewable energy. The combined use of District Heating Networks and Aquifer Thermal Energy Storage systems mitigates the variability of renewable energy production [1]. To evaluate the performance of the ATES-DHN systems, both aquifer-related and plant-related factors must be considered. Numerical simulations are the primary tool for investigating these parameters. DHN and ATES models are often simulated by different specific software, but to assess the global behavior of the integrated system, the DHN and ATES simulations should be coupled. The goal of this work is to study the impact of hydrogeological, thermal and energy parameters by coupling DHN and ATES simulations.

2. Materials and Methods

TRNSYS [2] simulates building thermal and cooling loads and plant action, while FEFLOW [3] models ATES behavior. At each timestep, TRNSYS considers ATES temperature and calculates the extracted flow rate based on the water–water heat pump's outlet temperature. FEFLOW uses the flow rate and the temperature coming from DHN to compute aquifer temperature distribution. The ATES system, heat pump, and DHN are modelled with realistic aquifer and buildings characteristics, which have been previously determined.

3. Results and Discussion

The coupling workflow constitutes a valuable component of the overall results. It enables comprehensive consideration of the interaction between the ATES system and the water-water heat pump activating the DHN: factors such as user type, site location, and plant configuration influence thermal load, which subsequently affects the aquifer. Simultaneously, the temperature of stored underground water impacts the parametrization of the user-plant system. The integration of the ATES and plant models is achieved through a dynamic exchange of simulation results (Fig.1). Specifically, MATLAB is used to manage the TRNSYS simulations, while Python oversees the FEFLOW simulations. At each timestep, the outputs from the TRNSYS model - such as the required flow rates and injection temperatures - are passed to the FEFLOW model. In turn, FEFLOW updates the aquifer temperature distribution and sends this information back to TRNSYS. This iterative process allows for a continuous and synchronized simulation, ensuring that both systems operate based on the most current data from one another. The coupled simulation approach is applicable to various ATES-DHN configurations, enabling the identification of optimal parameter settings for adopting such systems. The main factors that affect the integrated system are the aquifer hydraulic conductivity and aquifer hydraulic gradient. Elevated values of these parameters reduce ATES thermal storage capacity, as injected water disperses rapidly away from the wells serving the DHN plant, thereby decreasing thermal recovery rates. Additionally, system performance is affected by thermal load, and consequently, the configuration of the DHN. Situations where user type, site latitude, or elevation result in high thermal demands can lead to gradual thermal drift within the aquifer.



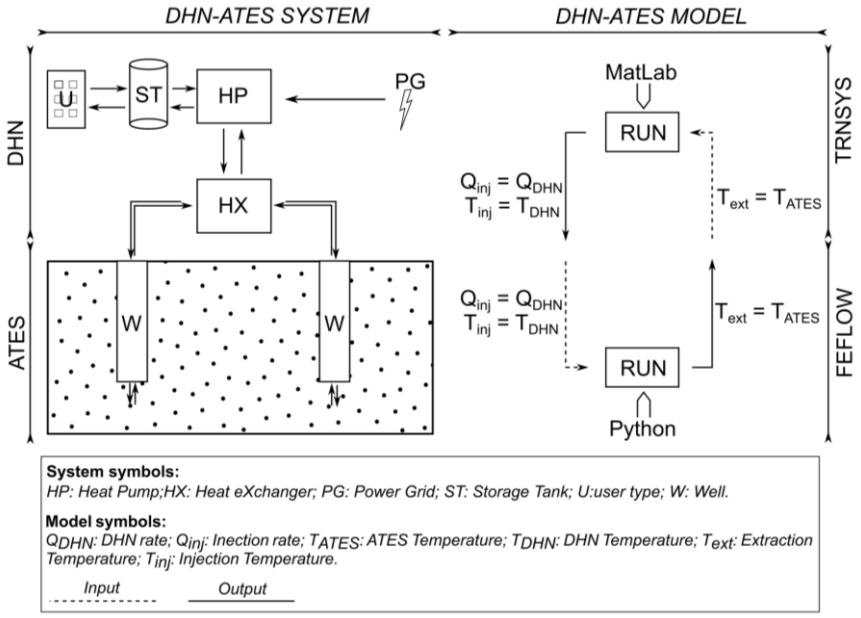


Figure 19 - Sketch of the DHN-ATES integrated system (on the left) and representation of the coupled modelling approach (on the right).

4. Conclusions

A coupled modelling approach has been developed to characterize the global behavior of integrated DHN-ATES systems. This method uses file exchanges between two distinct simulations, one for DHN dynamics and one for ATES processes. The output from each simulation serves as the input for the other. The performance of the integrated system depends on aquifer properties and building requirements, both of which are influenced by the specific site conditions.

Acknowledgements

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CLOSED-VESSEL EXPLOSION OF AMMONIA–HYDROGEN MIXTURES IN AIR - (C145)

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Keywords: ammonia–hydrogen mixtures, closed-vessel explosion behavior, industrial safety.

1. Introduction

Ammonia (NH_3), due to its high volumetric hydrogen density and chemical stability, has the potential to serve as a carbon-free hydrogen carrier, facilitating long-term storage and long-distance transport of renewable energy. It can be used either by extracting its stored hydrogen or directly as a fuel. However, direct combustion of NH_3 is hindered by high ignition energy and low reactivity. Enriching NH_3 with H_2 overcomes these limitations, inevitably increasing the risk of explosion. Effective risk mitigation requires a comprehensive understanding of the explosion behavior of NH_3–H_2 mixtures. Despite growing interest in these mixtures, quantitative explosion data—particularly under industrially relevant conditions and in comparison with the pure components—remain scarce [1–3].

In this work, explosion tests were conducted with NH_3, H_2, and an NH_3–H_2 mixture (H_2 mole fraction = 0.5) in a closed vessel at 250 °C, representing elevated operating temperatures, under an air atmosphere and at a fixed equivalence ratio of 1.1. Maximum pressure and maximum rate of pressure rise were extracted from the recorded pressure–time histories. The effect of NH_3–H_2 interactions on the mixture's explosion behavior is analyzed by direct comparison with the pure fuels.

2. Materials and Methods

The experimental activity was conducted in a closed-vessel explosion test facility, whose main component is a vertically oriented, 5 L cylindrical chamber (the vessel) with a length-to-diameter ratio of approximately 3, made of AISI 316 stainless steel. Pressure was recorded using a high-frequency transducer (150 kHz natural frequency) mounted at the top of the vessel, while gas temperature was monitored with a K-type thermocouple positioned at the center. Ignition was achieved via a high-voltage electric arc.

Pure NH_3, pure H_2, and NH_3–H_2 mixtures in air were prepared directly in the chamber using the partial pressure method. Air was added to reach an initial pressure of 1 bar. Prior to ignition, the chamber was heated to 250 °C using a controlled heating system, and a stirring device ensured that all prepared mixtures were homogeneous. Ignition was triggered after a short delay to allow turbulence to decay.

For the NH_3–H_2 mixture, the H_2 mole fraction was set to 0.5. The equivalence ratio was fixed at 1.1 for all fuels (NH_3, H_2, and the NH_3–H_2 mixture). Each test was performed at least three times to ensure reproducibility.



3. Results and Discussion

The peak explosion parameters, namely the maximum pressure, P_{max}, and the maximum rate of pressure rise, $(dP/dt)_{max}$, were extracted from the experimental pressure–time histories recorded for NH_3, H_2, and the NH_3–H_2 mixture (data not shown). The results are summarized in Table 1 as mean values ± standard deviations.

Table 1. Maximum pressure, P_{max}, and maximum rate of pressure rise, $(dP/dt)_{max}$, of NH_3, H_2, and the NH_3–H_2 mixture. Experimental conditions: 250 °C, 1 bar, air atmosphere, equivalence ratio = 1.1, H_2 mole fraction in the fuel mixture = 0.5.

Fuel	P_{max} [bar]	$(dP/dt)_{max}$ [bar/s]
NH_3	3.68 ± 0.04	32.98 ± 3.65
NH_3–H_2	4.07 ± 0.02	149.14 ± 3.48
H_2	4.39 ± 0.02	834.12 ± 23.72

H_2 exhibits much higher reactivity than NH_3, as evidenced by the dramatic increase in $(dP/dt)_{max}$. Specifically, the $(dP/dt)_{max}$ of H_2 is more than 25 times higher than that of NH_3, whereas P_{max} varies only modestly. This contrast highlights that $(dP/dt)_{max}$ is particularly sensitive to chemical kinetics, while P_{max} reflects the total energy effectively released in the system. The explosion behavior of the NH_3–H_2 mixture is bounded by the individual fuels, with both P_{max} and $(dP/dt)_{max}$ lying between the values of pure NH_3 and pure H_2. The measured $(dP/dt)_{max}$ of the mixture is well below the molar-weighted average of the pure fuels (149.14 versus 433.55 bar/s), showing strong antisynergistic effects. These results indicate that the mixture's explosion behavior cannot be inferred from the individual fuels alone, as the pressure dynamics are shaped by the interplay of their chemical reactivity.

4. Conclusions

In summary, NH_3 dominates the explosion behavior of the NH_3–H_2 mixture. Strong antisynergistic interactions between NH_3 and H_2 reduce the mixture's explosion severity, as evidenced by the measured $(dP/dt)_{max}$ lying well below the molar-weighted average of the pure fuels. These findings, quantified at an H_2 mole fraction in the fuel mixture of 0.5 and expected to qualitatively hold at lower fractions, provide a basis for developing effective strategies to mitigate the explosion risk of H_2-enriched NH_3 in industrial settings.

Acknowledgements

The authors acknowledge the financial support from the Italian national initiative "Research on the Electric System" (RdS) for the 2025–2027 implementation period, *Theme 1.3 Integrated Project on Technologies and End-Uses of Hydrogen*, funded by the Ministry of the Environment and Energy Security (MASE) through the Program Agreement with RSE S.p.A., ENEA, and CNR.

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ACTIVE MATERIALS FOR BIOFUEL CONVERSION IN HIGH TEMPERATURE ELECTROCHEMICAL CELLS - (C149)

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Keywords: ethylene, methane, solid oxide cell

1. Introduction

Solid oxide cell technology relies on the steady development of solid oxide fuel cells over the last four decades. Such devices are expanding their applications from power generation to a wider range of possible electrochemical reactions. In the context of increasing availability of renewable electricity such electrochemical reactors offer a powerful platform for the conversion of power and molecules by reactions in which the separation and selectivity of reactants and products can be controlled by the electrical potential. The range of possible reactions is broad if the different ionic species transported across the electrolyte, such as oxygen ions and protons, are coupled with catalytic active electrodes. Several important reactions for the decarbonization of key industrial processes, such as the direct conversion of methane to ethylene via de oxidative coupling, occur in the same temperature range of the operation of solid oxide cells. Thus, the present study demonstrates solid oxide cells using catalytic active layers for exploring power generation along with the production of industrially relevant molecules, such as syngas and ethylene.

2. Materials and Methods

Perovskites, with partially substituted cation by catalytic active metals, and doped-ceria fluorites are synthesized by chemical methods. Such oxides are compatible with standard zirconia-based solid oxide cells and are used as the catalytic layer in the fuel electrode for different reactions. The main advantage of such electrode configuration is to keep the industrially developed SOC components and use catalysts tailored for the desired products. The produced catalysts are initially screened in a fix-bed reactor, and the most active compounds are then applied to the solid oxide cell for electrochemical tests. Solid oxide cell tests are coupled with gas analysis systems to correlate the operating conditions and the produced species.

3. Results and Discussion

The results of cell voltage dependence on both applied current and methane concentration during CH_4 conversion in solid oxide cell with lanthanum-ceria based catalytic layer are presented in Figure 1. The experimental data shows stable operation with no signs of deactivation of the catalytic layer or degradation of the fuel cell, indicating satisfactory cell performance for the electrochemical oxidative coupling of methane process. The production of C2 compounds was accompanied by syngas (H_2+CO) and the cogeneration of electrical energy. At a fixed current density of 20 mA cm^{-2} at 850 °C the production rate for C2 and for H_2 are ~ 3 mmol min^{-1} cm^{-2} and 45 mmol min^{-1} cm^{-2}, respectively, with a H_2/CO ration ~1.7 Increasing current from 20 to 100 mA cm^{-2} increased the methane conversion from ~5% to 9%, whereas the C2 production rate considerably decreased.

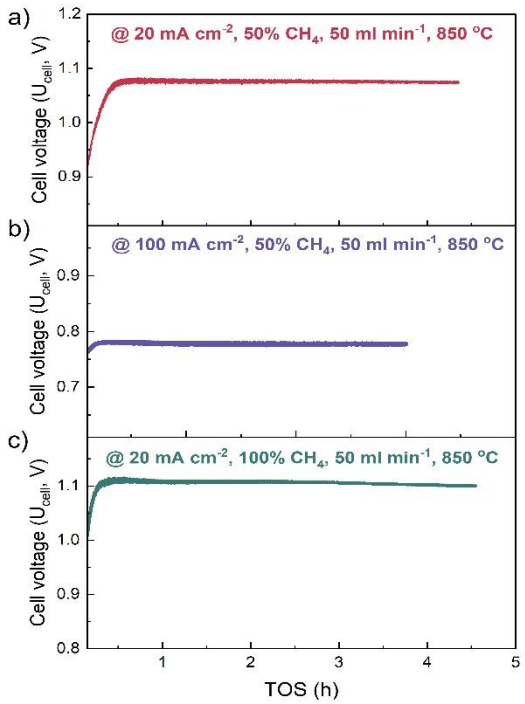


Figure 20. Cell voltage as a function of TOS for the Ca-doped $La_{0.5}Ce_{0.5}O_2$ layer in SOFC operating at 850 °C: (a) 20 mA cm^{-2}, 50% CH_4/He; (b) 100 mA cm^{-2}, 50% CH_4/He; and (c) 20 mA cm^{-2}, 100% CH_4. Total fuel flow =50 mL min^{-1}.

4. Conclusions

Using a catalytic layer expands the use of solid oxide cells to relevant reactions such as the oxidative coupling of methane. Solic oxide cells were demonstrated to produce a mixture of syngas and C2 compounds, along with a surplus of electricity. Catalyst development and tuning the operating parameters are key aspects to further advance such technology.

Acknowledgements

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ELECTROCHEMICAL WATER OXIDATION FOR IN-ORBIT HYDROGEN PEROXIDE PRODUCTION - (C150)

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Keywords: $2e^-$ water oxidation reaction; electrochemical H_2O_2 production, green propellants

1. Introduction

The electrochemical two-electron water oxidation reaction[1] ($2e^-$ WOR) has been investigated as a promising route for the decentralized production of H_2O_2. This research is central to the Green Solar-to-propellant Water Propulsion (Green SWaP) project, which aims to establish a sustainable method for producing propellants (H_2O_2 and H_2) directly in space. This approach enables low-cost, eco-friendly, and self-sufficient future space missions, facilitating safer and more efficient in-orbit services. To this end, electrochemical screening of various catalysts was performed to establish performance benchmarks necessary for developing the anode of a flow-cell for H_2O_2 production.

2. Materials and Methods

The preparation of catalysts (TiO_2 NTs, g-C_3N_4, 0.3%wtPd/N-CNTs, and the benchmark Degussa P25) followed previously described protocols.[2,3] For electrochemical characterization, catalysts were deposited as an ink onto glassy carbon (GC) electrodes 0.07 cm^2 (Amel 492/GC/3). Standard electrochemical (CV, LSV, and CA) measurements were carried out by using a Metrohm PGSTAT30 workstation in a three-electrode configuration: the catalyst deposited on GC tip served as WE, Pt wire as CE, and Ag/AgCl as a RE, whereas bi-distilled H_2O, 1M $KHCO_3$, and 0.1M NaOH were used as electrolytes. Generated H_2O_2 was quantified via $KMnO_4$ titration after 1-hour CA and the calculated yield of H_2O_2 reported in terms of mM/h.

3. Results and Discussion

The electrochemical performance of metal oxide catalysts (Degussa P25 and TiO_2 NTs) was compared with that of carbon-based catalysts (g-C_3N_4 and 0.3%wtPd/N-CNTs) in the 2e-WOR for H_2O_2 electrosynthesis with different electrolytes. Potentiometric measurements (CV, LSV, and CA) show that 1M $KHCO_3$ yields the highest oxidation currents compared to 0.1 M NaOH and bi-distilled H_2O. Figure 1(a) shows the LSV curves recorded for each catalyst in different electrolyte, which highlighting the onset potentials and oxidation currents. Figure 1b) reports the amounts of H_2O_2 produced in 1-h CA experiments with different catalysts and electrolytes. Finally, to study the effect of applied potential, a 1-hour CA experiment was conducted at 3.2 V and 2.4 V_{RHE} for the 2e-WOR reaction and the amounts of H_2O_2 produced in each case were compared (see Figure 1c). For the TiO_2 NTs catalyst, at 3.2 V_{RHE}, a H_2O_2 concentration of 2.75 mM was detected after 15 minutes of reaction, and this concentration remained constant for up to 1 hour of accumulation. When the potential was lowered to 2.4 V_{RHE}, H_2O_2 production increased sharply for up to 45 minutes, reaching a maximum concentration of 5.3 mM, a 1.93-fold increase compared to the values recorded at the higher potential. This suggests that the system is more favourable for the 2e-WOR pathway, which allows for greater H_2O_2 production, at lower applied potentials. Conversely, at higher potentials, the competitive reaction (OER) is favoured, and significant oxygen evolution was observed on the anode surface. At the same time, H_2O_2 decomposition may also occurs. Therefore, optimizing the applied potential is essential to increase the H_2O_2 yield in this electrochemical process. Moreover, all the catalyst tested have been investigated in



dark conditions, then considering their absorption properties in the UV-Vis region, we expect further improvements performing the experiments under solar light illumination.

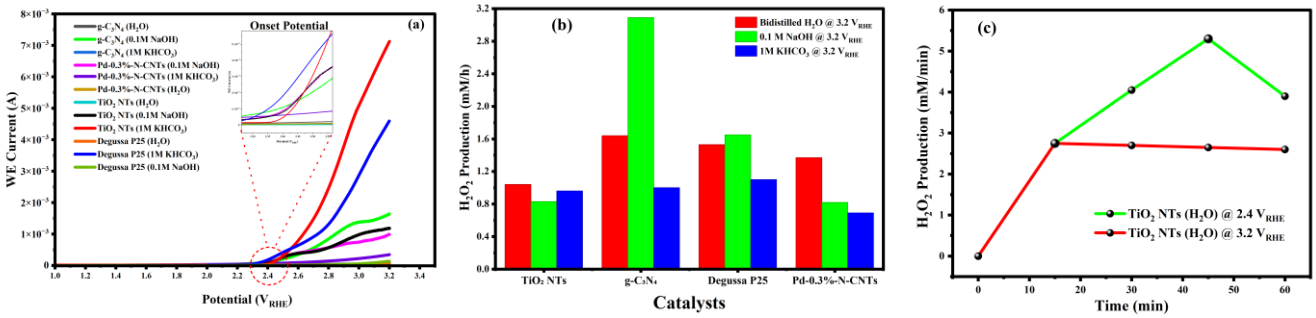


Figure 1. a) LSVs of the investigated catalysts; b) amounts of H_2O_2 obtained in 1-h CA with different catalysts and electrolytes; c) 1-h CA on TiO_2 NTs at different potentials highlighting the role of potential in favouring H_2O_2 path formation.

4. Conclusions

All the investigated catalysts exhibited promising performance in H_2O_2 production. g-C_3N_4 showed the highest activity in alkaline medium, at higher potential ($3.2V_{RHE}$) whereas TiO_2 NTs maximized H_2O_2 selectivity at lower potentials ($2.4V_{RHE}$). This confirms that operating at lower applied potentials can favour H_2O_2 electrosynthesis — depending on the catalyst and reaction conditions — by promoting the $2e^-$ pathway while simultaneously limiting H_2O_2 decomposition. These findings highlight the potential of these catalysts for space-grade H_2O_2 production. Ongoing work focuses on improving anode stability and validating TRL-4 operation under flow-cell conditions.

Acknowledgements

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ENERGY CONSUMPTION ANALYSIS AND LIFE CYCLE ASSESSMENT OF A LI-ION BATTERY PACK FOR A LOWER-LIMB ASSISTIVE EXOSKELETON - (C151)

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Keywords: Li-ion, battery pack, energy consumption, LCA.

1. Introduction

Exoskeletons are wearable devices designed to support human movement and reduce physical effort in applications such as rehabilitation, industry and assistive care. Among the main design requirements, these devices must be lightweight and capable of ensuring all-day operation [1]. For this reason, increasing attention is being devoted to the selection of the power supply system, as it is one of the components that most strongly affects both weight and autonomy. Lithium-ion batteries are currently the most common solution [2]; however, their capacity is directly linked to pack size, so longer operating time generally results in increased mass. In this context, alternative power supply systems for exoskeletons, particularly hybrid fuel cell–battery architectures, should be investigated to identify the best compromise in terms of weight, autonomy, and size. This study presents the energy consumption analysis of a lower-limb exoskeleton for elderly assistance in subjects with muscular weakness and, based on this, the design and prototyping of a battery pack. In addition to technical performance, a preliminary Life Cycle Assessment is included to evaluate environmental sustainability. While the literature mainly identifies limited autonomy and high weight as the main drawbacks of battery-only systems, this work also investigates whether environmental impact should be considered an additional limitation. Future work will include comparison with the hybrid system and an economic analysis.

2. Materials and Methods

A full lower-limb assistive exoskeleton with four actuated joints (bilateral hip and knee) was designed for home use to support elderly and sarcopenic individuals with muscle weakness during daily domestic activities. The energy consumption of walking, sit-to-stand, stand-to-sit, slope and stairs was estimated through experimental tests on two subjects. These activities were then combined into a representative daily-use scenario reflecting the typical needs of an elderly user in a domestic environment. For the battery pack realization, Panasonic NCR18650B cells were selected. The life cycle assessment (LCA), carried out using SimaPro software, considered the materials and equipment involved throughout the entire manufacturing process, as well as the use phase of the device.

3. Results and Discussion

Figure 1 shows the energy analysis for each activity.

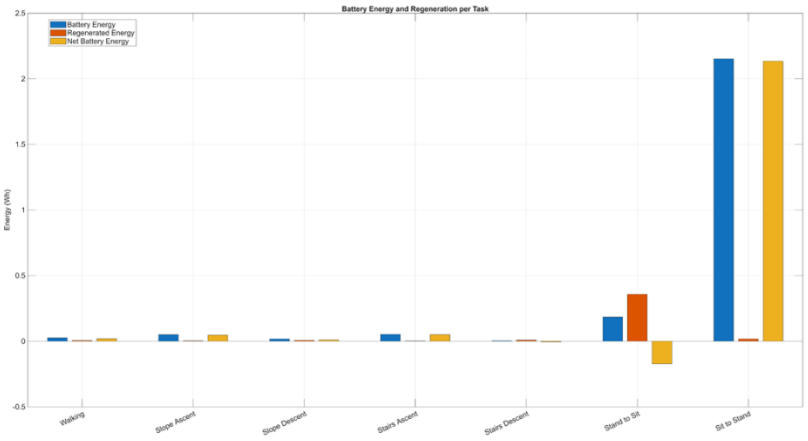


Figure 1. Energy analysis of exoskeleton's tasks.

Considering a daily-use scenario, approximately 200 Wh with no energy recovery strategy are required. Potential recovery mechanisms could provide an energy gain up to 50 Wh, partially reducing the total battery demand.

Based on these results, a 10S2P lithium-ion battery pack was selected. With a nominal voltage of 36 V, the pack provides 234 Wh and a capacity of 6.5 Ah, representing a feasible compromise between energy availability and system integration. From an environmental perspective, the preliminary LCA was included to extend the assessment beyond technical performance alone and to explore the potential environmental implications of the battery pack.

4. Conclusions

This work presented the energy consumption analysis, design, and prototyping of a lithium-ion battery pack for a lower-limb assistive exoskeleton. The estimated energy demand for a representative daily-use scenario was evaluated together with the potential contribution of regenerative strategies. Based on these results, a battery pack configuration was identified as a suitable solution for the considered application. The preliminary LCA helped clarify the role of environmental sustainability in exoskeleton battery-pack design and provided a first framework for integrating environmental considerations into future developments. These results provide the baseline for future comparison with a hybrid fuel cell–battery system, which will also be assessed from environmental and economic perspectives.

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STOICHIOMETRIC CONTROL OF CO-SPUTTERED $BiVO_4$ THIN FILMS FOR ENHANCED PHOTOELECTROCHEMICAL WATER OXIDATION - (C154)

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Keywords: Bismuth Vanadate, Magnetron Sputtering, Photoelectrochemical, Stoichiometry, Water Splitting.

1. Introduction

Efficient photoelectrochemical (PEC) water splitting requires optimized metal-oxide photoelectrodes. Bismuth Vanadate ($BiVO_4$) is a leading candidate due to its 2.4 eV bandgap; however, performance is highly sensitive to cation stoichiometry [1,2]. Current research often relies on complex doping or nano structuring [3] to overcome poor charge transport. This work addresses the under-explored role of precise stoichiometric control in magnetron-sputtered systems. We demonstrate a scalable co-sputtering route to tune the Bi/V ratio. The novelty lies in isolating stoichiometry as the primary driver for phase stabilization and PEC enhancement, providing a robust pathway for high-performance $BiVO_4$ photoanodes without extrinsic dopants.

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2. Materials and Methods

$BiVO_4$ films were fabricated via reactive magnetron co-sputtering using independent metallic Bi and V targets. Stoichiometry was tuned by varying V-target power while maintaining constant Bi power, yielding Bi/V ratios from 0.73 to 1.39. Structural evolution was characterized by XRD and Raman spectroscopy. PEC performance was evaluated in 0.5 M Na_2SO_4 under AM 1.5G illumination to determine photocurrent density and Half-Cell Solar-to-Hydrogen (HC-STH) efficiency.

3. Results and Discussion

Analysis confirms that phase-pure monoclinic scheelite $BiVO_4$ is only stable within a narrow stoichiometric window. Deviations lead to secondary phases ($Bi_4V_2O_{11}$ or V_2O_5) that act as recombination centers. The optimized near-stoichiometric film achieved a photocurrent density of 1.95 mA/cm² at 1.23 *V vs RHE* and a maximum HC-STH of 0.27%. Efficiency gains are attributed to improved bulk charge transport and interfacial kinetics. Notably, the band gap remained stable at ~2.42 eV across the series, confirming that performance shifts are electronic/structural rather than optical. This demonstrates that near-perfect cation balance minimizes intrinsic defects that otherwise limit carrier lifetime in sputtered oxide films.



Bi/V Atomic Ratio	Primary Phase	Photocurrent (mA/cm^2)	Band Gap (eV)
0.73 (V-rich)	BiVO4+V2O5	0.85	2.41
1.02 (Optimal)	Monoclinic BiVO4	1.95	2.42
1.39 (Bi-rich)	BiVO4+Bi4V2O11	0.62	2.43

Table 1. *Effect of Bi/V atomic ratio on the phase composition, photocurrent density, and optical band gap of bismuth vanadate photoanodes*

4. Conclusions

We established that precise stoichiometric control is a stand-alone strategy for enhancing $BiVO_4$ photoanodes. By eliminating secondary phases through co-sputtering power regulation, we achieved performance approaching the limits of undoped systems. This scalable, industrially relevant fabrication route simplifies the production of high-efficiency photoelectrodes for hydrogen generation. Future work will explore the integration of these films into tandem devices for bias-free water splitting.

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FUNCTIONALIZED MEMBRANES BASED ON POLY(2,6-DIMETHYL-1,4-PHENYLENE)OXIDE (PPO) - (C155)

with Tunable Micro and Macroporosity: Structural Features and Applications

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Keywords: Nanoporous Crystalline phases, Transparent and Flexible films, Sulfonated PPO films, Pollutant sorption, Molecular sensors

1. Introduction

In this communication, we report on the structural features of Nanoporous Crystalline (NC) phases in syndiotactic polystyrene (s-PS) and poly(2,6-dimethyl-1,4-phenylene) oxide (PPO) (1-3).

A general methodology for the fabrication of High Surface Area (HSA) PPO films will be presented. These films achieve specific surface area values as high as 620 m²/g, maintaining such performance across a wide thickness range, from a few micrometers up to several hundreds of microns (4,5). We discuss an innovative approach to the development of multifunctional PPO films characterized by a hydrophilic sulfonated amorphous phase and a physically crosslinked hydrophobic crystalline phase (6-8). This dual-phase architecture offers a promising strategy for balancing chemical functionality with structural stability in advanced polymeric membranes.

2. Materials and Methods

Films showing both NC phases and microporosity , as well as sulfonated NC PPO films were obtained as described in refs (3-8). All samples were characterized WAXD analysis, with a Bruker D8 diffractometer.

3. Results and Discussion

A general methodology for achieving polymeric films presenting nanoporous crystalline (NC) phases for two commercial polymers such as syndiotactic polystyrene (s-PS) and poly(2,6-dimethyl-1,4-phenylene) oxide (PPO) will be shown. The main feature of NC phases is their lower density than the corresponding amorphous phases, which leads to the high uptake of organic guest molecules, even when they are present only in traces.

We present preparation procedures leading to High Surface Area PPO and sPS films with SA higher than 600 $m^2\ g^{-1}$ and 120 $m^2\ g^{-1}$ 1, respectively. Due to the presence of mesopores beside the micropores of their crystalline phases, HSA NC films can be opaque and exhibit poor toughness, and hence, can be unsuitable for some applications. Furthermore, we identify specific crystallization conditions that yield HSA PPO films with transparency and toughness comparable to their amorphous counterparts. These HSA, transparent, and tough NC PPO films are expected to be suitable for many applications where these properties are needed (Figure 1).

Moreover, the ability of high-SA NC PPO films to remove organic molecules from air and water by studies on sorption and desorption kinetics for a relevant pollutant, perchloroethylene (PCE) will be presented. Due to their rapid pollutant uptake, coupled with high thermal and mechanical stability, these novel HSA NC PPO films are poised for diverse applications in environmental remediation, molecular separations, and chemical sensing.



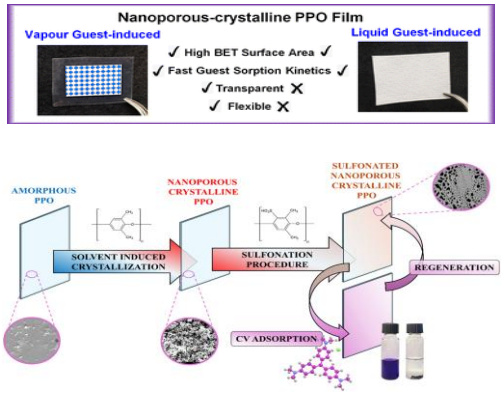


Figure 21: Digital photos of NC PPO films, a schematic representation of their functionalization and application for dye removal.

Finally, an innovative method to produce PPO films featuring a hydrophilic sulfonated amorphous phase and a physically crosslinked hydrophobic crystalline phase is discussed, highlighting their potential as advanced materials for molecular sensors and water purification (6-8). The capability of -SO3 functionalized PPO, as nanoporous crystalline polymer, as adsorbent materials for the removal of cationic dyes such as crystal violet, methylene blue and rhodamine B from wastewater will be also presented.

4. Conclusions

An efficient route to obtain transparent, high-surface-area nanoporous crystalline films of s-PS and PPO was achieved. These materials demonstrated fast and efficient uptake of organic pollutants from water (PCE); sulfonated PPO enables selective removal towards cationic pollutants. This communication proves the efficient applications of NC films in different fields (environmental remediation, separation, sensing, etc.).

Acknowledgements

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LABORATORY-SCALE STUDY OF METHANE/BIOGAS PYROLYSIS IN MOLTEN SALTS – (C157)

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Keywords: Hydrogen, Pyrolysis, Molten Chlorides, Methane, Biogas

1. Introduction

Methane pyrolysis represents a viable method to produce hydrogen with zero CO_2 emissions, according to the following reaction:

$CH_{4(g)} \leftrightharpoons C_{(s)} + 2H_{2(g)}$

By this process, the methane molecule is decomposed into its elements, obtaining hydrogen as a fuel and, ideally, solid carbon as the only byproduct. To date, several approaches are proposed for this route, including thermal catalytic, non-catalytic and plasma processes, and bubbling the gaseous reactants in high-temperature liquid baths. The latter methodology is very promising, given it allows the segregation of carbon on the melt surface, and provides excellent heat transport inside the reactor. Among the possible molten media considered for this process, salt mixtures present several advantages with respect to metals, thanks to their lower density, which leads to a minor pressure drop for the gas phase across the reactor, and good solubility in water, which allows an easier separation of the produced carbon.

2. Experimental

A quinary chloride mixture was selected among other options based on its thermo-physical properties, freezing point and density, which were evaluated through experimental and modelling methods. A laboratory-scale setup was developed for the experimental study the pyrolysis reaction (Figure 1), using two different quartz reactor geometries. Mass flow meters and controllers were employed to set the reactor feed. Pure methane and a mixture of methane and carbon dioxide (50:50 v:v)) where used to simulate biomethane and biogas, respectively. A Varian 4900 micro-chromatograph was placed downstream the reactor to evaluate the outlet gas composition. Condensable subproducts were dissolved in cyclohexane and analyzed by a gas chromatograph (Agilent 7890A). equipped with a HP MS5 (30m) column, and a mass spectrometer detector. Table 1 summarizes the conditions for the performed experimental campaign.



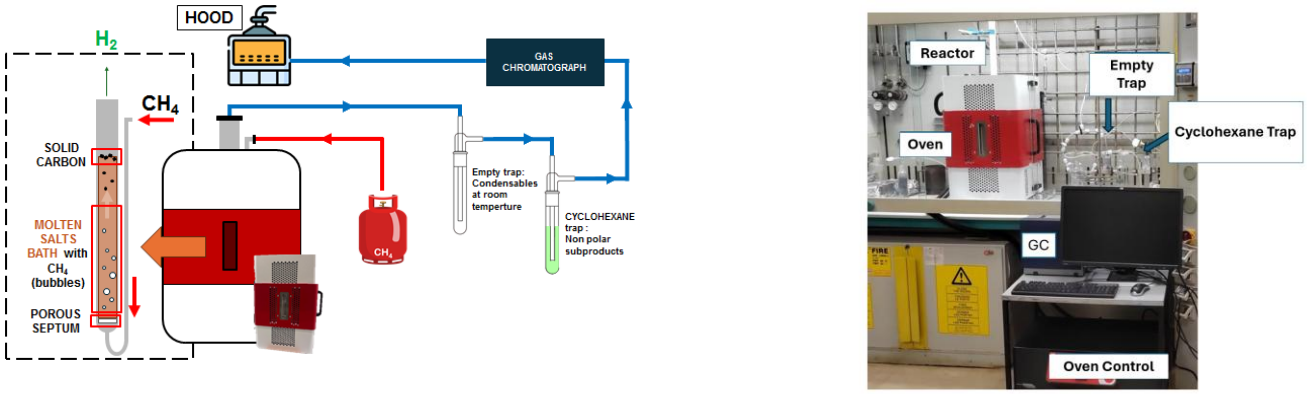


Figure 1. On the left and right, respectively, a scheme and a picture of the laboratory scale experimental set-up was for pyrolysis in molten chlorides

Table 1. Summary of the experimental tests

TEST ID	CH_4 mass flow [Nml/min]	CO_2 mass flow [Nml/min]	Temperature [°C]	Reactor geometry
A1	32	0	600-700-800	#1
A2	32	0	800	#1
B	25	0	800-900	#1
C1	30	30	500	#2
C2	50	50	600-700	#2
D	68-51-34	0	600-700-800	#2

4. Results

An example of the obtained results is represented in Figure 2.



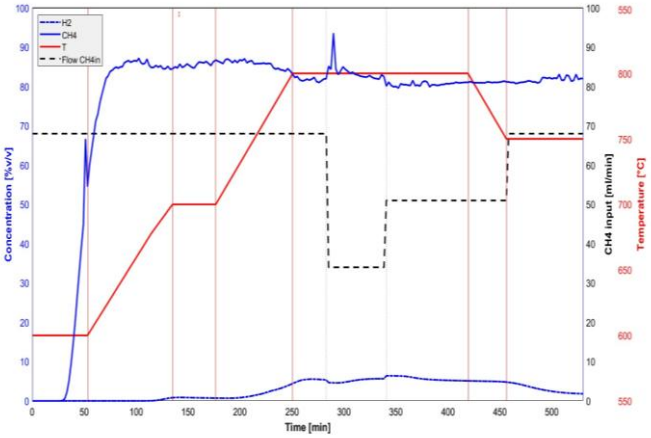


Figure 2. Hydrogen and methane outlet concentrations, temperature and methane inlet mass-flow as a function of the reaction time.

Appreciable methane conversions are present starting from 600°C; above 800°C, also ethane, ethylene and acetylene are detectable, together with PAH, which are condensable at room temperature. When a CH_4/CO_2 mixture is fed to the reactor, only carbon is produced but the amount of hydrogen became nearly undetectable under the conditions considered in the tests.

Some major issues were identified, mostly related to the salt mixture volatility and zinc reduction by methane and hydrogen, which are currently being addressed.

Acknowledgements

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EUROPEAN PROJECT FUNDED C3POE : SUSTAINABLE PLUG & PLAY WATER ELECTRICITY COUPLING FOR ISLANDS AND ISOLATED COASTAL SITES OPTIMAL DESIGN OF AN OFF-GRID HYBRID RENEWABLE ENERGY SYSTEM INVOLVING BATTERIES, HYDROGEN AND PRODUCING WATER AND ELECTRICITY - (C161)

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Keywords: Smart Grids, Renewable energy, Storage, Batteries, Hydrogen

1. Introduction

This study focus on grid-independent water and electricity production system based on hydrogen and battery storage coupled with renewable energy production from a mix of photovoltaic solar and wind power. The system's operation is simulated at a time resolution of one hour, based on energy production data deduced from meteorological conditions on the island of Molène in Brittany in western France. The model calculates the energy and water management and starts to consider ageing and replacement of main components. The sizing approach emphasizes the importance of meteorological and load input data, based on a Pareto front analysis obtained from a multi-objective optimization algorithm. Several photovoltaic-wind energy mix scenarios are studied. Input data from 2018 to 2023 are used to discern the impact of favorable and unfavorable meteorological and load conditions on the sizing results.

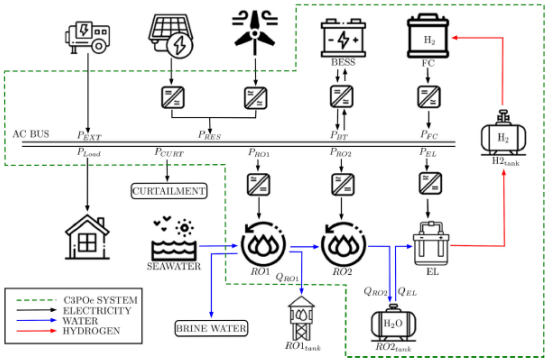


Figure 1. Schematic diagram of the C3POe system, with connection of the various sub-systems to the water, electricity and hydrogen networks.



2. Materials and Methods

A shortage indicator has been defined to assess the suitability of each year's data set for each scenario. This indicator is based on a simplified energy management system. It can be interpreted as a means of assessing the mismatch between renewable energy production and consumption. Renewable energy production $ERES(t)$ is intermittent, so some of it can be distributed directly to the user, stored inside a storage system, or lost. As users' energy consumption $ELoad(t)$ is difficult to predict, the energy has to be provided either directly from the RES, or from the storage system, or from an external source $EEXT(t)$.

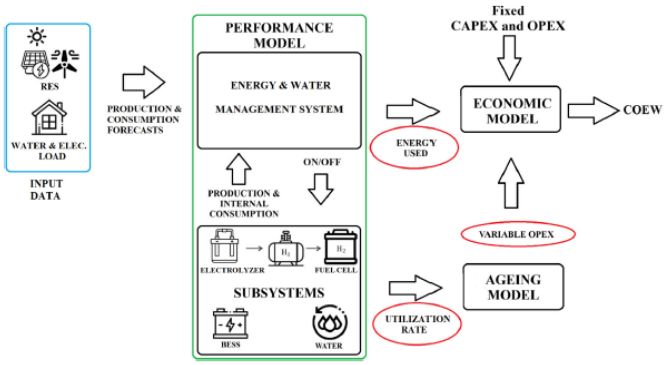


Figure 2. Simplified diagram of the model used to determine the cost of the energy and water produced.

3. Results and Discussion

This sequence of calculations illustrates that sizing based on fixed input conditions does not guarantee an energy cost, but gives an approximation of it. This is essential for validating parameters, but also for testing system flexibility. In the overall dimensioning approach, the minimum and maximum values of COEW and $EEXTELoad$ has to be considered to determine the choice of a parameter set.

4. Conclusions

Looking forward, several avenues for future research are identified. More detailed physical models of key subsystems (electrolyzer, fuel cell, battery, and RO unit) could be incorporated to better reflect ageing effects and dynamic behavior. In addition, substantial renewable energy surpluses were observed, which suggests the potential for integration of flexible, on-demand applications such as wastewater treatment, heat production, or desalination. A comprehensive sensitivity analysis is planned to assess the impact of modeling assumptions.

Acknowledgements

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WASTE-TO-FUEL: EFFICIENT CONVERSION OF PLASTIC WASTE TO METHANE VIA CATALYTIC HYDROGASIFICATION IN AN OPTIMIZED REACTOR CONFIGURATION - (C163)

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Keywords: plastic waste, hydrogasification, methane production, structured catalyst.

1. Introduction

Rapid economic growth and rising living standards are accelerating the depletion of fossil fuels. To limit environmental pollution and meet growing energy needs, the development of alternative and sustainable energy sources, like carbonaceous materials, is essential. In particular, the catalytic conversion of plastic waste offers a promising route to recover a resource that would otherwise accumulate in landfills. Among the conversion methods, hydrogasification stands out: it is exothermic, requires no added oxygen, produces methane suitable for blending with natural gas, and can reach thermal efficiencies up to 80%. Studies on coal hydrogasification identify iron-group metal catalysts as the most effective, especially when combined with basic promoters like calcium to limit coke formation and sulfur poisoning [1, 2].

2. Materials and Methods

The catalyst was prepared using an OBSiC open-cell foam carrier, coated with a γ-Al_2O_3 washcoat, a CeO_2 layer, and Ni and Ca phases. Characterization included N_2 physisorption and Hg intrusion porosimetry, SEM-EDX, H_2-TPR and CO_2-TPD. Experimental tests were carried out in a 2 L reactor equipped with independently heated zones and designed to process up to 100 g of plastic. A mass spectrometer was calibrated in order to provide methane concentration in the product stream.

3. Results and Discussion

Experimental tests confirmed the feasibility of this approach, with methane production increasing with the amount of plastic waste fed to the reactor and reaching a plateau of around 50 vol.% (Figure 1). Quantitative analysis of the gas stream showed that, at a plastic-to-catalyst ratio of 1.5, the process yielded approximately 450 Nm^3 of gas per ton of plastic waste, with 405 Nm^3 of methane and 16 kg of hydrogen consumed. Methane is the main product, accounting for approximately 84-89% of the total gas, which is much higher with respect to the methane yield in conventional plastic gasification/pyrolysis systems currently employed..

As expected from the nature of the feedstock and despite the promotional effect of calcium on nickel, coke formation was observed, underscoring the need for effective regeneration strategies. The catalysts were regenerated and tested in a subsequent experimental test where they exhibited well-preserved activity, as the methane production reaching peak values in the range of 500–570 $NmL \cdot min^{-1}$, comparable to the ones reported with the fresh catalyst. Moreover, the values of methane production normalized per ton of plastics and grams of active phase are relatively close (55 for the fresh catalyst and 51 $Nm^3_{CH4} \cdot ton_{plastic}^{-1} \cdot g_{cat}^{-1}$ for the regenerated), which reinforces the conclusion that the catalyst preserves its functional performance after regeneration.



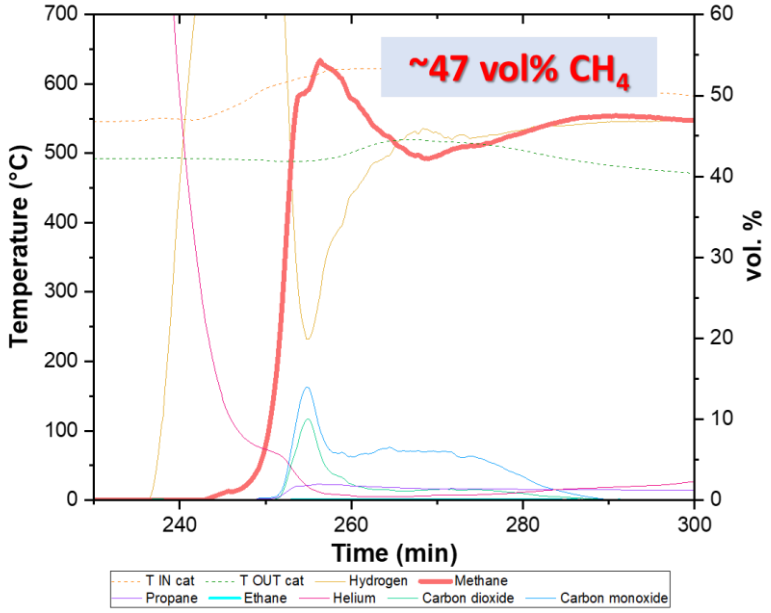


Figure 1. Details of the results of the test with 105 g of plastic waste.

4. Conclusions

This work demonstrates the feasibility of converting plastic waste into methane through catalytic hydrogasification. Tests with up to 105 g of feed produced methane concentrations up to 59 vol%, with a stable plateau around 50 vol%. Hydrogen consumption was 16 $kg \cdot ton^{-1}_{plastic\ waste}$, and gas yield reached 450 $Nm^3 \cdot ton^{-1}_{plastic\ waste}$, with methane at 89%. Some coke formed, partially damaging the OBSiC foam, but regeneration restored catalyst activity, indicating no significant deactivation.

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NEAR-AMBIENT CO_2 ACTIVATION WITH ULTRA-HIGH METHANE SELECTIVITY - (C164)

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Keywords: Cold Plasma, low temperature CO_2 activation, Optical Emission Spectroscopy, Plasma-catalyst interaction, high methane selectivity

1. Introduction

Cold Plasma-assisted CO_2 hydrogenation utilizes non-thermal plasma (NTP) to activate CO_2 and H_2 under mild conditions, enabling highly selective methane synthesis even at low temperatures. Because this is an exothermic equilibrium reaction, it naturally releases heat, hence it would be optimal to operate at low temperatures. Traditional thermal plants rely on burning fossil fuels to reach the high temperatures necessary to overcome activation energy barriers, a process that is not only environmentally damaging due to high CO_2 emissions but also thermodynamically counterproductive for exothermic yields. NTP solves this by using energetic electrons to induce vibrational and electronic excitation, producing reactive species while keeping the gas bulk phase at lower temperatures. This bypasses the "heat-yield trade-off" and eliminates the reliance on fossil-fuel combustion. When the NTP system is not thermally insulated, it suffers from low selectivity. Without insulation, the reactor is prone to heat dissipation and internal temperature gradients which result in the “freezing” of the reaction intermediates, which are no longer able to undergo the subsequent steps to obtain methane. By incorporating proper insulation, we stabilize the reaction environment and ensure that the plasma energy is channeled specifically into the intended pathway, maximizing the purity of the synthesized methane.

2. Materials and Methods

A structured catalyst consisting of 10% wt. Ni on sepiolite has been obtained through the wet impregnation method. It has then been characterized with different physicochemical analyses in order to evaluate its textural properties. Experiments were conducted in a Dielectric Barrier Discharge (DBD) reactor integrated with the Ni-Sepiolite catalyst, which was previously tested in a thermal setup to assess its activity towards Sabatier reaction. The research focused on optimizing the reactor layout and the operating conditions to increase CO_2 conversion and, most importantly, CH_4 selectivity. The impact of space velocity and thermal insulation were assessed. Furthermore, a parametric analysis was performed on the reactant mixture composition by varying Argon dilution.

3. Results and Discussion

NTP assisted tests showed the possibility to obtain appreciable CO_2 conversion levels at as low as 40 °C reaching the maximum values at temperatures up to 100 °C lower than the ones needed with the thermal setup. However, a low CH_4 selectivity is encountered, which could be due to the “freezing” of reaction intermediates. Said intermediates are not able to undergo the subsequent hydrogenation reactions since a part of the energy of the system is dissipated as heat by the system. The results highlight that reactor insulation is a determining factor in preventing said quenching, allowing for unit selectivity and high yields at mild temperatures (230-240 °C).



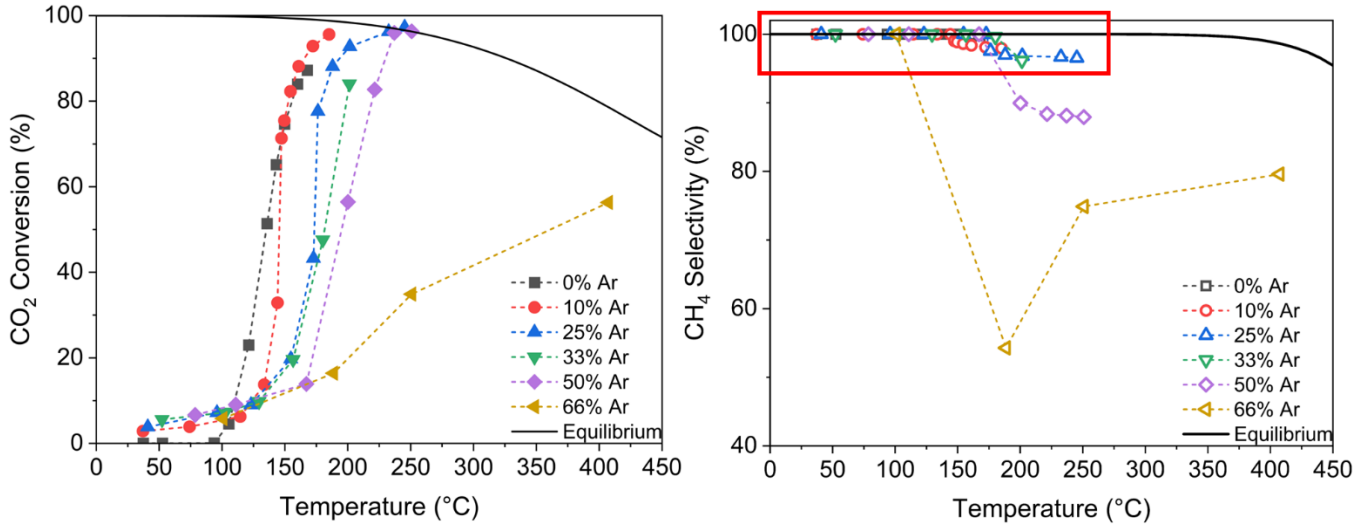


Figure 22 CO_2 conversion and CH_4 selectivity of Non-Thermal Plasma tests with different feed compositions.

The most significant finding concerns the elimination of the carrier gas: operating with an almost pure mixture (10% Ar), the system achieved methane yields exceeding 93% utterly reducing the temperature at which these yields have been achieved. These tests have been carried out at a space velocity of 0.5 NL/(g_{cat}h) with power inputs ranging from 8 W to 36 W. Most importantly, the elimination of carrier gas resulted in a considerable increase in terms of CH_4 selectivity which in the case of the lowest Ar-containing mixtures, never dropped below 99.7%. Hence, although Argon works as a promoter for the NTP discharge it also subtracts energy which would ensure the carrying out of the subsequent hydrogenation reactions necessary to transform the CO(v) obtained thanks to the dissociation of the CO_2 into CH_4.

4. Conclusions

The study successfully demonstrates that the synergy between non-thermal plasma (NTP) and a Ni-Sepiolite catalyst effectively bypasses the thermodynamic limitations of conventional methanation. The findings reveal that thermal insulation is essential to prevent the quenching of reaction intermediates, enabling near-unit selectivity at temperatures significantly lower than traditional thermal processes. Crucially, the research proves that eliminating Argon dilution—while seemingly counterintuitive for discharge stability—actually maximizes energy efficiency and methane yield by preventing energy loss to the carrier gas. These results establish a highly efficient, carrier-free operational framework that is both economically and technically viable for the industrial scale-up of Power-to-Gas systems.

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DIMENSIONLESS FRAMEWORK FOR CO_2 SPLITTING IN DBD PLASMA REACTORS - (C165)

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Keywords: DBD plasma reactors, CO_2 splitting, Plasma-assisted conversion, Plasma chemistry.

1. Introduction

Dielectric barrier discharge (DBD) reactors are attracting increasing attention for plasma-assisted CO2 conversion because they operate under mild conditions and can be directly coupled with renewable electricity. However, despite extensive studies on electrical diagnostics and reactor performance, predictive scaling criteria for reactor comparison and design are still lacking [1–3]. Conventional descriptors such as specific energy input (SEI) capture global trends but do not explicitly separate electrical forcing, convective transport, and chemical conversion. In this work, a dimensionless framework for DBD CO_2 splitting is proposed by combining Masuda, Reynolds, and Damköhler numbers to rationalize the coupled electro-chemo-fluid behavior of the reactor.

2. Materials and Methods

A coaxial alumina-based DBD reactor operated with pure CO_2 was experimentally investigated under different plasma powers, gas flow rates, discharge gaps, and reactor lengths. Electrical observables were extracted from Lissajous figures, while CO_2 conversion and energy efficiency were determined from outlet gas analysis. Dimensionless groups were calculated to correlate electrical and performance descriptors under varying operating conditions.

3. Results and Discussion

Electrical observables derived from the Lissajous analysis showed a dominant dependence on plasma power and reactor geometry, while reactor performance was strongly affected by gas throughput and residence time. The Masuda number successfully organized the scaling of voltage-related discharge descriptors, highlighting the role of electro-fluid forcing. In parallel, the Damköhler number correlated with conversion and energy efficiency, confirming the relevance of transport–reaction competition.

The combined electrohydrodynamic descriptor N·Da, where N = Md/Re, provided an improved collapse of the experimental data by simultaneously accounting for electrical forcing, convection, and chemical conversion. Figure 1 shows that both CO2 conversion and energy efficiency follow coherent trends when represented through this coupled dimensionless parameter. Additional comparison with literature datasets demonstrated that the proposed framework remains applicable across different reactor geometries and operating conditions, supporting its use as a transferable engineering correlation for DBD plasma reactors.



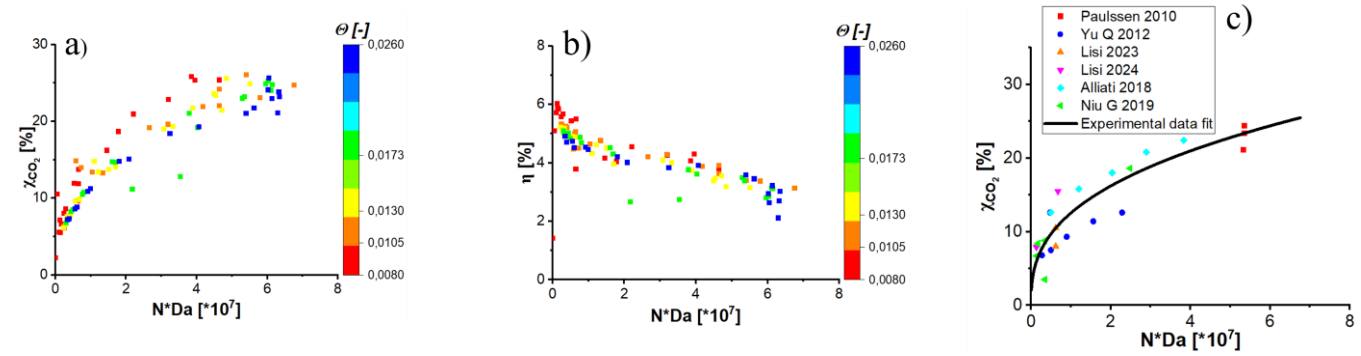


Figure 23: Experimental CO_2 conversion (a) and energy efficiency (b) against the coupled electro-chemo-fluid parameter N·Da; (c) CO_2 conversion vs N·Da for combined literature datasets at T_g = 150 °C.

4. Conclusions

The proposed dimensionless framework provides a physically interpretable description of DBD plasma reactors for CO2 splitting by separating and coupling electrical forcing, convective transport, and chemical conversion. The combined use of Masuda, Reynolds, and Damköhler numbers improves the organization of reactor behavior beyond empirical SEI-based analysis and offers a promising basis for reactor comparison, optimization, and scale-up.

Acknowledgements

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METHANOL PRODUCTION FROM CO_2 HYDROGENATION OVER Cu SUPPORTED ON BLACK-TiO_2 - (C166)

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Keywords: methanol synthesis, CO_2 hydrogenation, oxygen vacancies

1. Introduction

CO_2 emissions are among the primary drivers of climate change, making its reduction in the atmosphere an urgent global priority [1]. A promising strategy involves the valorization of CO_2 as a feedstock for the production of biofuels, such as methanol, thereby transforming a waste product into a valuable resource. Methanol synthesis is a catalytic process that requires optimized formulations to maximize process yields. The conventional industrial catalyst is $Cu/ZnO/Al_2O_3$; however, recent studies have shown that supports characterized by oxygen vacancies enhance CO_2 adsorption and activation, thereby improving the overall efficiency of the process. Accordingly, this study focuses on the use of Cu-ZnO catalysts supported on black titania, which possesses a high concentration of surface oxygen vacancies that enhance CO_2 adsorption and activation efficiency [2].

2. Materials and Methods

The samples were prepared through a two-step procedure: (i) synthesis of black titania ($bTiO_2$) via high-temperature reduction under an inert atmosphere using $NaBH_4$ as the reducing agent; (ii) introduction of the copper phase through a liquid-phase impregnation step followed by chemical reduction at room temperature, again employing $NaBH_4$ as the reducing agent.

The Cu/black titania catalysts were characterized by Raman spectroscopy, UV–Vis spectroscopy, CO_2 temperature-programmed desorption (CO_2-TPD), and specific surface area (SSA) evaluation.

Catalytic tests were carried out in a stainless-steel tubular reactor, where the catalyst bed was positioned between two layers of glass wool. The CO_2/H_2 feed mixture was supplied at a 30/70 ratio, with a weight hourly space velocity (WHSV) of 10 h^{-1}, under pressures ranging from 1 to 20 bar and temperatures between 180 and 300 °C. The outlet stream was subsequently analyzed by mass spectrometry.

3. Results and Discussion

The catalytic results provided clear evidence of the key role played by oxygen vacancies in CO_2 hydrogenation. A preliminary experimental test was carried out to evaluate their influence by comparing the catalytic performance of Cu/TiO_2 and $Cu/bTiO_2$. The results showed that the catalyst based on non-reduced titania did not exhibit any detectable methanol formation under the investigated conditions. In contrast, the $Cu/bTiO_2$ sample led to measurable methanol production, highlighting the crucial contribution of oxygen vacancies in promoting CO_2 adsorption and activation, and consequently enhancing hydrogenation activity.

Subsequently, the effect of copper loading was investigated by comparing two catalysts, $15Cu/bTiO_2$ and $30Cu/bTiO_2$, containing 15 wt% and 30 wt% Cu, respectively. The results indicated no substantial differences in catalytic performance between the two samples, suggesting that increasing the copper content beyond 15 wt% does not significantly improve methanol synthesis under the tested conditions.



On this basis, a further catalyst was developed by incorporating ZnO into the 15Cu/bTiO₂ system. This choice was motivated by literature reports identifying the Cu–ZnO interface as the primary active phase for CO_2 hydrogenation to methanol [3]. Indeed, the addition of ZnO resulted in a marked increase in methanol selectivity and methanol TOF, demonstrating the beneficial synergy between oxygen-deficient black titania and the Cu–ZnO active phase.

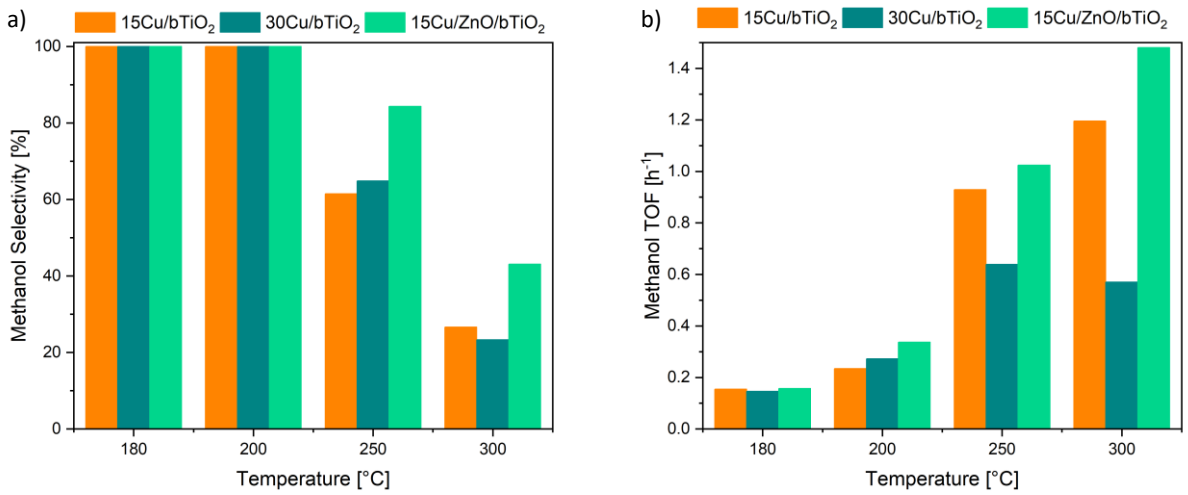


Figure 24 Comparison of the tested catalysts as a) Methanol Selectivity, and b) Methanol TOF at 20 bar and WHSV = $10h^{-1}$

4. Conclusions

The results demonstrate that oxygen vacancies in black titania play a decisive role in promoting CO_2 hydrogenation to methanol. While increasing Cu loading does not significantly enhance performance, the introduction of ZnO markedly improves methanol selectivity. These findings highlight the synergistic effect between oxygen-deficient supports and Cu–ZnO active sites.

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AMMONIA CRACKING ELECTRIFIED STRUCTURED REACTOR COUPLED WITH PEM FUEL CELL FOR POWER GENERATION - (C167)

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Keywords: Ammonia Cracking, Joule Heating, Ni-based Catalyst, Structured Catalyst, Energy Efficiency.

1. Introduction

Modern chemical industry prioritizes energy transition to green processes, focusing on two main pillars: (I) alternative energy sources and (II) sustainable heating. Regarding the former, hydrogen is a compelling alternative to conventional fossil fuels. However, significant challenges persist concerning its transport and storage. Consequently, ammonia has emerged as a promising carbon-free hydrogen carrier. [1] Regarding the latter, the electrification of endothermic reactions offers a sustainable substitute for traditional combustion-based heating. Among various electrification techniques, Joule heating has demonstrated significant potential for industrial applications. [2, 3]

This work investigated catalytic ammonia cracking via Joule heating as a pathway for green hydrogen production.

2. Materials and Methods

Four OB-SiC foams were employed as carrier for the structured catalyst, which featured a catalytic formulation of 24%Ni/30%CeO_2-70%Al_2O_3. The foams were coated with an alumina washcoat via dip-coating, while Ceria (30%) and Nickel (24%) were loaded through wet impregnation, using Cerium(III) Nitrate Hexahydrate and Nickel(II) Nitrate Hexahydrate as precursors. The catalysts were subsequently calcined at 700°C. The catalyst was characterized via 77K nitrogen adsorption, mercury intrusion porosimetry and temperature-programmed reduction (TPR). Heating was achieved by Joule effect, utilizing a resistance in intimate contact with the catalyst (**Errore. L'origine riferimento non è stata trovata.**). The catalyst efficacy was assessed by NH_3 conversion, while the energy consumption was quantified in terms of $KWh/Nm^3_{prod.\ H_2}$.

3. Results and Discussion

Both 77K nitrogen adsorption and mercury intrusion porosimetry confirm a significant increase in surface area and porosity following the washcoating process. TPR analysis, conducted up to 650°C (10% H_2/Ar at 5°C/min), evidenced high dispersion of the active phase and a complete reduction of Nickel Oxide to metallic Nickel. Catalytic performance was evaluated across a temperature range of 250-650°C and pressures of 1-7bar, utilizing a feed of 50vol% of NH_3 (Argon balanced), at varying weight hourly space velocities (WHSV).

To assess the energy efficiency of the Joule Heating system, experimental energy consumption was compared against theoretical values, calculated as the enthalpy difference between the inlet and outlet gas streams. The results demonstrated good catalytic activity, achieving near-complete conversion below 600°C with an activation temperature of approximately 300°C. Regarding energy efficiency, the system attained an efficiency of about 70%.

The results concerning both the catalytic and the energy performance are highly significant in the framework of energy transition toward hydrogen as a primary fuel. The implementation of Joule heating enables a substantial reduction in reactor footprint, supporting the ultimate objective of integrating ammonia cracking units with hydrogen fuel cells or hydrogen-powered engines.



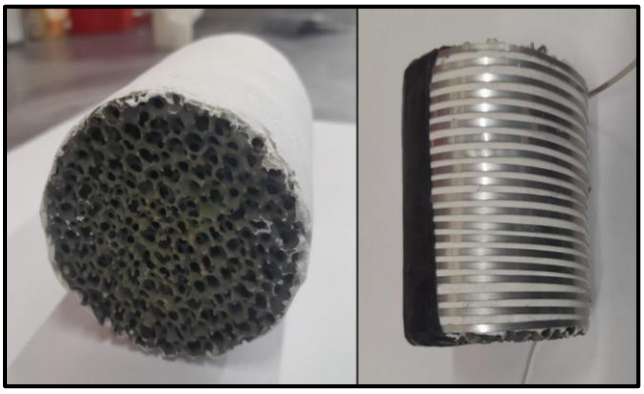


Figure 25 A batch of four OB-SiC foams loaded with 24%Ni/30%CeO_2-70%Al_2O_3, assembled and electrified using a kanthal flat wire.

4. Conclusions

This study focused on the development and evaluation of a Ni-based structured electrified catalyst, supported by CeO_2-Al_2O_3. The catalyst demonstrates superior performance compared to Ni-based catalyst previously reported in the literature. Notably, the energy efficiency attained represents one of the most significant results to date for Joule Heating applied to the Ammonia Cracking. Future research will explore strategies to further optimize this efficiency.

Acknowledgements

This research was funded by PROGETTI DI RICERCA DI RILEVANTE INTERESSE NAZIONALE – Bando 2022 PNRR Prot. P2022BEWCZ "AMmonia-Based electrIfied processes inTegrated wIth fuel cells for pOwer generatioN - (AmBition)". The authors thank Eng. R. Trifone and Eng. F. Milone for the experimental support.

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HYDROGEN PRODUCTION VIA AMMONIA CRACKING REACTION: IMPACT OF SUPPORT MATERIAL ON CATALYTIC PERFORMANCE - (C168)

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Keywords: Powder Catalysts, Ammonia Cracking, Hydrogen Production, Ni-based, Support Materials.

1. Introduction

The modern chemical industry prioritizes the energy transition through green processes. In this context, Hydrogen is a leading solution, due to its high gravimetric energy density and its versatility. However, the primary limitation of utilizing hydrogen as an energy carrier remains the challenges associated with its transport and storage. Currently, chemical hydrogen carriers represent a compelling alternative. Ammonia is one of the most promising carbon-free options, due to its established infrastructure for transport and storage.

This study investigates a series of Ni-based powder catalysts, with a specific focus on the influence of different support materials on catalytic performance of the ammonia cracking reaction. [1, 2]

2. Materials and Methods

Four distinct supports were employed to prepare a set of catalysts with different nickel concentrations.

The used supports were γ-alumina (γ-Al_2O_3), mesoporous silica (SiO_2), cerium aluminate (CeO_2-Al_2O_3) and hydrotalcite (HTC). Specifically, the CeO_2-Al_2O_3 support was prepared by wet impregnation of γ-Al_2O_3. All catalysts, featuring Ni concentration between 3 and 24wt%, were prepared by wet impregnation, using Nickel(II) nitrate hexahydrate as the precursor, dried at 120°C and calcined at 700°C for 1 hour, with a heating ramp of 10°C/min. The powders were characterized via 77K nitrogen adsorption, mercury intrusion porosimetry and temperature-programmed reduction (TPR). The catalysts' performance was evaluated in terms of ammonia conversion.

3. Results and Discussion

Characterization via 77K nitrogen adsorption and mercury intrusion porosimetry revealed that HTC-supported catalysts possessed a significantly lower specific surface area (SSA), which negatively impacted catalytic activity. In contrast, mesoporous silica exhibited both a substantially higher SSA and larger mean pore dimensions.

TPR was performed under a reducing mixture up to 650°C and a ramp of 10°C/min, with a total flow rate of 300 NmL/min consisting of 5vol% hydrogen and 95vol% argon. All catalysts show characteristic Ni peaks and the TPR analysis confirms the complete reduction for all the samples investigated.

Catalytic tests were carried out at room pressure, within a temperature range of 250-650°C, using a 50vol% NH_3 (Ar balanced), by varying weight hourly space velocity (WHSV) from 3.3 h^{-1} to 5.5 h^{-1}. The study demonstrated that while support pore dimension positively influences ammonia conversion, this effect diminishes at higher active phase loading. Specifically, at 24wt% Ni, the positive effect of the mesoporosity of the SiO_2 became less pronounced. Conversely, the CeO_2-Al_2O_3 support, despite its lower SSA, showed superior catalytic performance at high Ni loadings, as illustrated in **Errore. L'origine riferimento non è stata trovata.**.



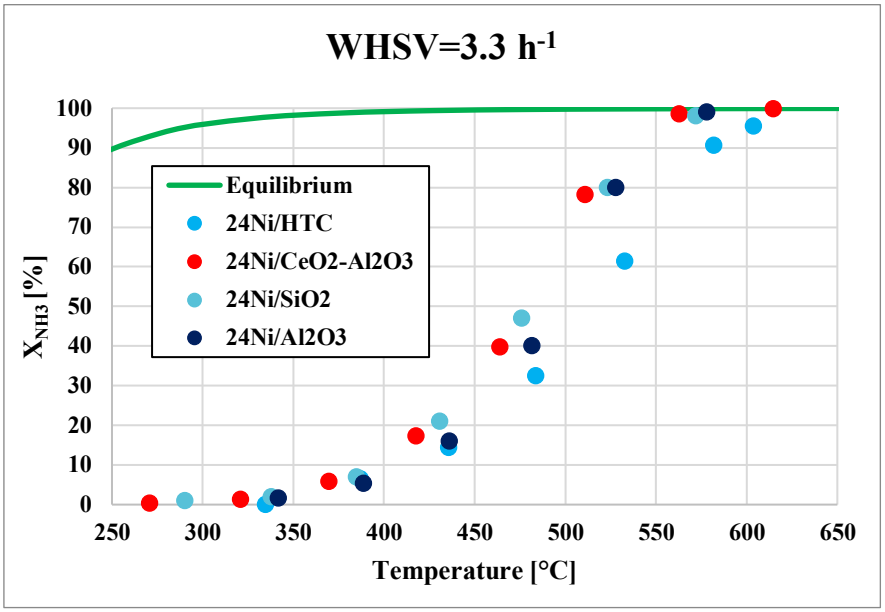


Figure 26 Comparison of the catalytic performance for 24wt% Ni catalysts, by varying the support at WHSV=3.3h^{-1}.

4. Conclusions

This work investigated the influence of four different supports on the performance of Ni-based catalysts for the ammonia cracking reaction. At a nickel concentration of 24wt%, the CeO_2-Al_2O_3 support yielded the highest catalytic performance. The study further underscores the critical role of support selection and contact time in optimizing ammonia conversion. Future research will focus on exploring alternative active phases, aiming to reduce the total conversion temperature below 500°C.

Acknowledgements

This research was funded by PROGETTI DI RICERCA DI RILEVANTE INTERESSE NAZIONALE – Bando 2022 PNRR Prot. P2022BEWCZ "AMmonia-Based electrIfied processes inTegrated wIth fuel cells for pOwer generatioN - (AmBition)". The authors thank Eng. Trifone and Eng. Visconti for the experimental support.

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ENHANCING SELECTIVITY TO PROPYLENE IN THE PROPANE DEHYDROGENATION PROCESS BY JOULE-HEATED PT-SN BASED CATALYTIC FOAMS - (C169)

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Keywords: Propane dehydrogenation, Joule heating, Structured catalysts, Process intensification, Energy efficiency.

1. Introduction

To address the limited propylene selectivity, the rapid deactivation of the catalyst, and the high energy demand challenges of the propane dehydrogenation (PDH) reaction, this study explores the electrification of the process via Joule heating. Traditional PDH reactors rely on an external heating mode through fossil fuel combustion, which results in an inefficient radial thermal gradient with hotter regions near the reactor wall that promote homogeneous side reactions. This work aims to overcome these limitations by using structured catalysts that simultaneously act as resistive heating elements, employed to reverse the heat flux direction, enabling rapid and selective heat transfer directly to the active sites and improving both thermal management and process efficiency [1].

2. Materials and Methods

A Pt-Sn/MgAlO catalytic formulation was deposited over SiSiC periodic open cell structures (POCS). The structured catalysts were electrified using ring-shaped nickel-plated copper connections and tested for the PDH reaction under both conventional external heating and Joule heating modes. Axial thermal profiles were recorded using electrically insulated K-type thermocouples inside a purpose-designed steel reactor. Operating under severe conditions (80 vol% C_3H_8), the study evaluated single/dual-foam architectures and feed preheating strategies to suppress inlet thermal quenching and optimize the global energy balance.

3. Results and Discussion

As shown in Figure 1, Joule heating significantly improved PDH performance by inverting the radial thermal gradient and selectively supplying heat directly to the catalyst. This configuration enabled rapid and uniform catalyst heating while maintaining lower reactor wall temperatures, thereby suppressing gas-phase side reactions and coke formation. As a result, propylene selectivity above 99% was achieved at 570 °C, corresponding to an approximately 6% absolute increase compared with conventional external heating.

Energy balance analysis revealed that the baseline single-foam configuration achieved an overall efficiency of 36%. The implementation of a dual-foam architecture improved the thermal distribution along the reactive zone and reduced the specific energy consumption, increasing the efficiency to 55%. A further enhancement was obtained by mitigating inlet thermal quenching through feed preheating. By optimizing the residence time and balancing kinetic and thermodynamic limitations, the thermal energy introduced with the preheated feed was effectively converted into chemical work, resulting in a record overall efficiency of 61%.

Compared with previous electrified PDH technologies, such as microwave-assisted systems limited by magnetron efficiency, Joule heating demonstrated superior energy performance under equivalent reaction conditions [2]. The obtained efficiency exceeds the values currently predicted for electrified PDH reactors, highlighting the strong potential of Joule-heated structured catalysts for sustainable propylene production [3].



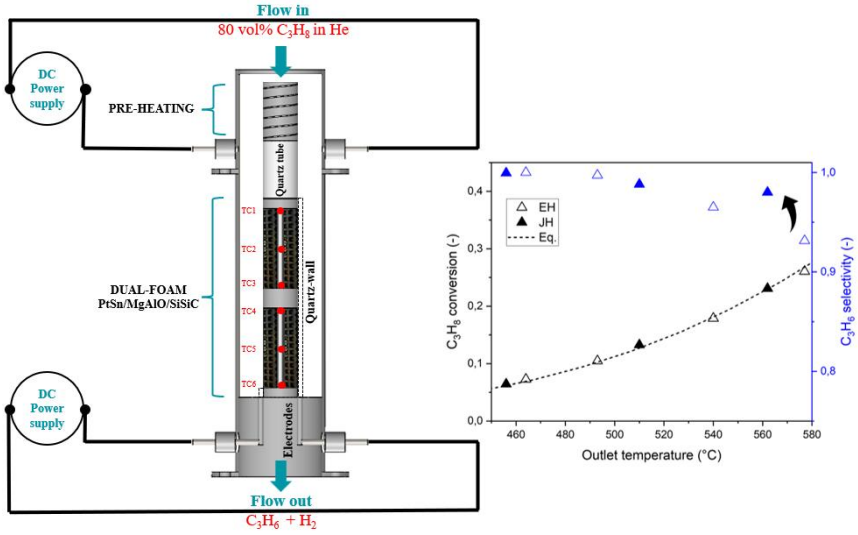


Figure 1: Scheme of the Joule-heated dual-foam catalytic reactor with pre-heating (on the left); results of the PDH activity tests with both Joule and traditional external heating in terms of C_3H_8 conversion and C_3H_6 selectivity (7 h^{-1} WHSV, 80 vol% C_3H_8 in He, 1 atm)

4. Conclusions

The strategic coupling of Joule heating, dual-foam architecture and feed preheating redefines the thermodynamic limits of PDH, achieving a record 61% energy efficiency at 10 h^{-1}. This confirms electrified structured reactors as a highly sustainable pathway for propylene production. Future work will explore distributed feeding strategies to precisely tailor the local thermal input, further advancing the industrial scale-up of this technology.

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LOW TEMPERATURE H_2 PRODUCTION BY HLC CRACKING IN ELECTRIFIED STRUCTURED REACTORS INTEGRATED WITH SUPPORTED Pd MEMBRANE - (C171)

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Keywords: Hydrogen liquid carriers; Ammonia cracking; Methanol steam reforming; Electrified structured reactors; Open-cell SiC foams; Pd membranes; Hydrogen production.

1. Introduction

The transition toward a hydrogen-based energy system requires efficient technologies for hydrogen production, storage, and distribution. Hydrogen Liquid Carriers (HLCs), such as ammonia and methanol, have emerged as promising alternatives for the safe transport and storage of hydrogen due to their high hydrogen content, established infrastructure, and ease of handling. However, the development of compact and energy-efficient reactors capable of releasing hydrogen at relatively low temperatures remains a key technological challenge [1, 2].

This work presents an innovative reactor concept based on electrically heated structured catalysts integrated with hydrogen-selective Pd membranes for the low-temperature ammonia cracking and methanol reforming. The proposed approach combines process electrification and membrane-assisted reaction engineering to enhance hydrogen productivity while reducing thermal losses and reactor carbon footprint.

2. Materials and Methods

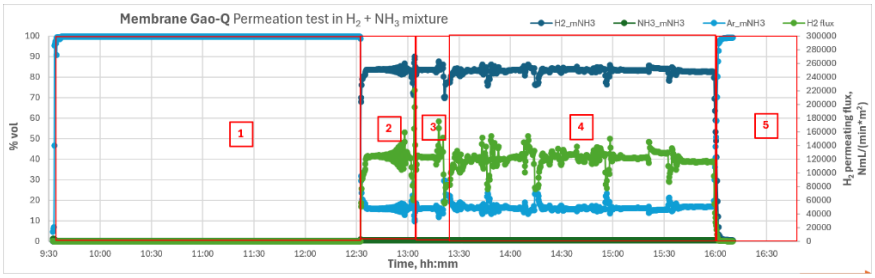
The reactor configuration employs highly conductive open-cell SiC foams (OBSiC, FOSECO) as structured catalyst supports, enabling efficient Joule-heating-assisted operation and excellent temperature uniformity. For ammonia cracking, Ni-based catalytic formulations are considered, while Pd–Cu catalysts supported on structured substrates are investigated for methanol steam reforming. Hydrogen separation is achieved through supported palladium membranes manufactured by GaoQ (China), consisting of a thin Pd layer deposited on a porous ceramic support, with external and internal diameter of 12.4 and 10 mm, respectively.

The effects of the main operating variables, including reaction temperature (350–550 °C), electrical power input, space velocity, pressure, feed composition, steam-to-carbon ratio in methanol reforming, and membrane permeation conditions, have been investigated.

3. Results and Discussion

Preliminary studies have been devoted to verifying the compatibility of the membrane with ammonia-containing streams. The results reported in Figure 1 demonstrated the excellent and stable hydrogen permeation performance of these membranes even in presence of ammonia (comparison between step 2, 3 and 4 in figure 1), making them particularly attractive for membrane-assisted ammonia cracking applications.





	1		2		3		4		5	
	Sweep gas side	Process gas side	Sweep gas side	Process gas side	Sweep gas side	Process gas side	Sweep gas side	Process gas side	Sweep gas side	Process gas side
P, bar	1	**1->5**	1	**5**	1	**3**	1	**2-3**	1	**1**
T, °C	RT->400	RT->400	400	400	400	400	400	400	400-> RT	400-> RT
Tot Flowrate, NmL/min	400	**1000**	400	**2476**	400	**2507**	400	**1000**	400	**1000**
Gas comp.	Sweep gas side	Process gas side	Sweep gas side	Process gas side	Sweep gas side	Process gas side	Sweep gas side	Process gas side	Sweep gas side	Process gas side
Ar	100%	0%	100%	0%	100%	0%	100%	0%	100%	0%
N2		100%		25%		0%		0%		100%
H2		0%		75%		74,07%		74,07%		0%
NH3		0%		0%		2,60%		2,60%		0%
He		0%		0%		23,32%		23,32%		0%

Figure 27 Preliminary hydrogen permeation tests with ammonia-containing streams.

Early tests were also carried out to investigate the feasibility of the electrified methanol reformer without membrane. The electrified system displayed an energetic efficiency of 55% under the typical operating temperatures of Pd-based membranes (450°C), offering a valid energy-efficiency alternative in the field of electrified hydrogen production.

4. Conclusions

In this work particular attention has been devoted to the synergistic interaction between reactor electrification, structured catalyst geometry, and continuous hydrogen extraction through the membrane. The selective removal of hydrogen is expected to shift the thermodynamic equilibrium toward higher conversion levels, enabling efficient operation at significantly lower temperatures than those required in conventional reactors. The proposed technology represents a promising pathway toward compact, highly efficient, and electrically driven hydrogen production systems suitable for distributed applications and future renewable-energy-powered hydrogen infrastructures.

Acknowledgements

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COST AND ROBUSTNESS OF OPTIMIZED CROSS-MEDITERRANEAN GREEN–BLUE HYDROGEN SUPPLY CHAINS UNDER 2050 POLICY SCENARIOS - (C174)

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Keywords: Renewable energy production, Hydrogen transport, MILP optimization, Techno-economics

1. Introduction

Dedicated hydrogen pipelines are expected to play a key role in large-scale European hydrogen transmission by 2050, complementing near-term blending strategies [1,2]. The European Hydrogen Backbone foresees a network linking renewable-rich regions, including North Africa, with European demand centers [3,4,5]. Corridor A aligns with GW-scale hydrogen plans in Tunisia, targeting up to 8.3 Mt/y by 2050, with Gabès and Cap-Bon acting as potential hubs connected to the Trans-Mediterranean Pipeline [6,7,8].

2. Materials and Methods

Figure 1 schematizes the hydrogen valley configurations, including PV, wind farms, PEM electrolysers, SMR+CCS, BESS, hydrogen storage, compression, desalination and pipeline transport. The study assumes a constant hydrogen supply of 1.35 MtH_2/year, equal to 30% of Corridor A demand. Five scenarios are assessed: Blue, Green and three Hybrid cases. A MILP framework minimizes LCOH while ensuring continuous supply, supported by dynamic pipeline simulation for compression requirements. The hydrogen supply chain is completed by a dynamic model of downstream distribution networks developed in MATLAB-Simulink, to assess the impact of variable hydrogen off-take profiles and mitigate pressure oscillations.

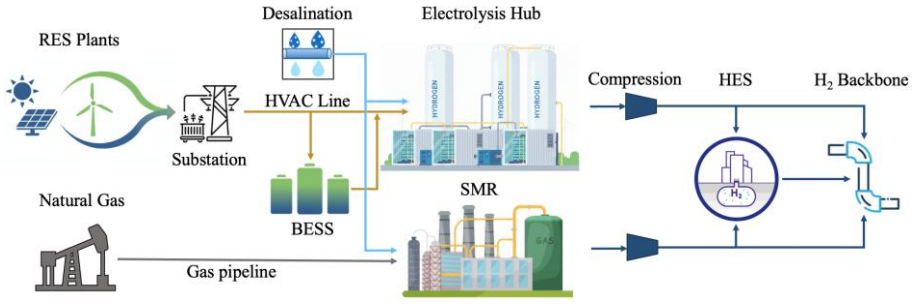


Figure 28. Schematic representation of the different hydrogen valley configurations

3. Results and Discussion

Figure 2 shows the optimal installed capacity of RES, electrolysis, BESS and SMR for the base-case scenarios. The total installed capacity increases almost linearly with the green hydrogen share. In the Green scenario, the system reaches 32.9 GW of RES, 17.1 GW of electrolysis and 7.5 GW of BESS power capacity, corresponding to 30 GWh of storage.



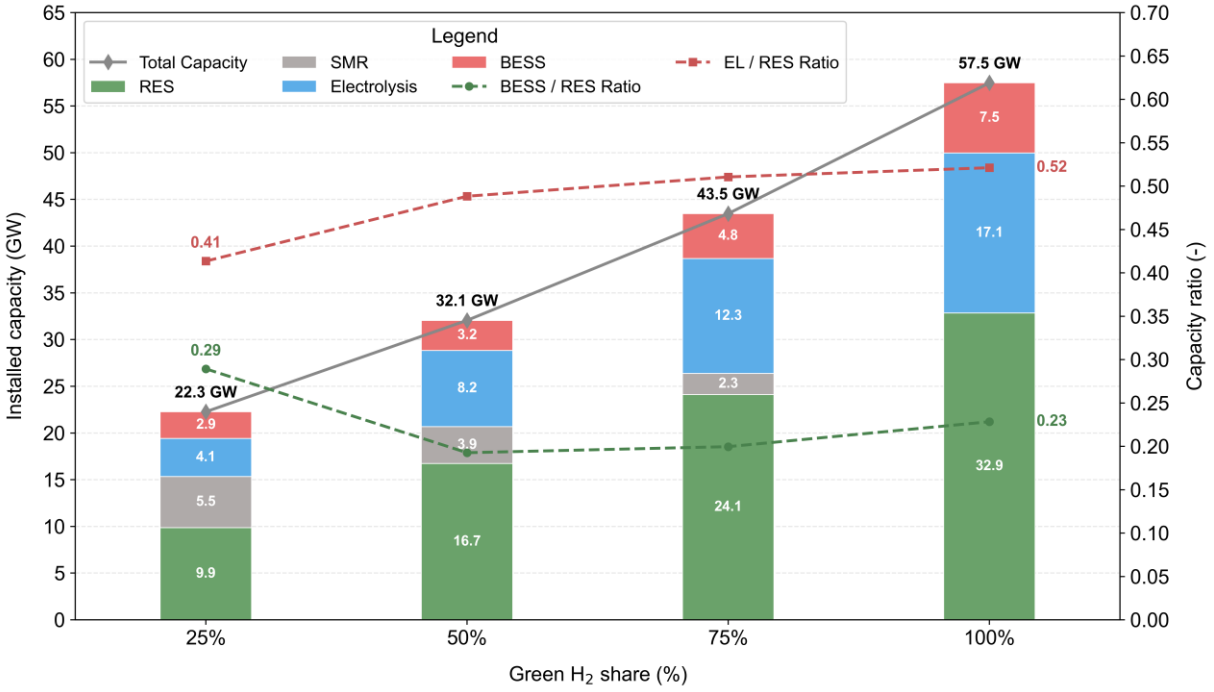


Figure 29. Optimal system sizing for Green and Hybrid base-case scenario

Figure 3 reports the optimal RES mix. PV dominates in all scenarios, representing about 74–84% of total RES capacity, followed by onshore wind at 15–23%, while offshore wind remains marginal at 1–3%. This is mainly due to the high solar productivity of the selected PV areas and their shorter average distance from the Gabès hub compared with wind sites. Nevertheless, wind capacity remains necessary to partially cover electricity demand during night hours.

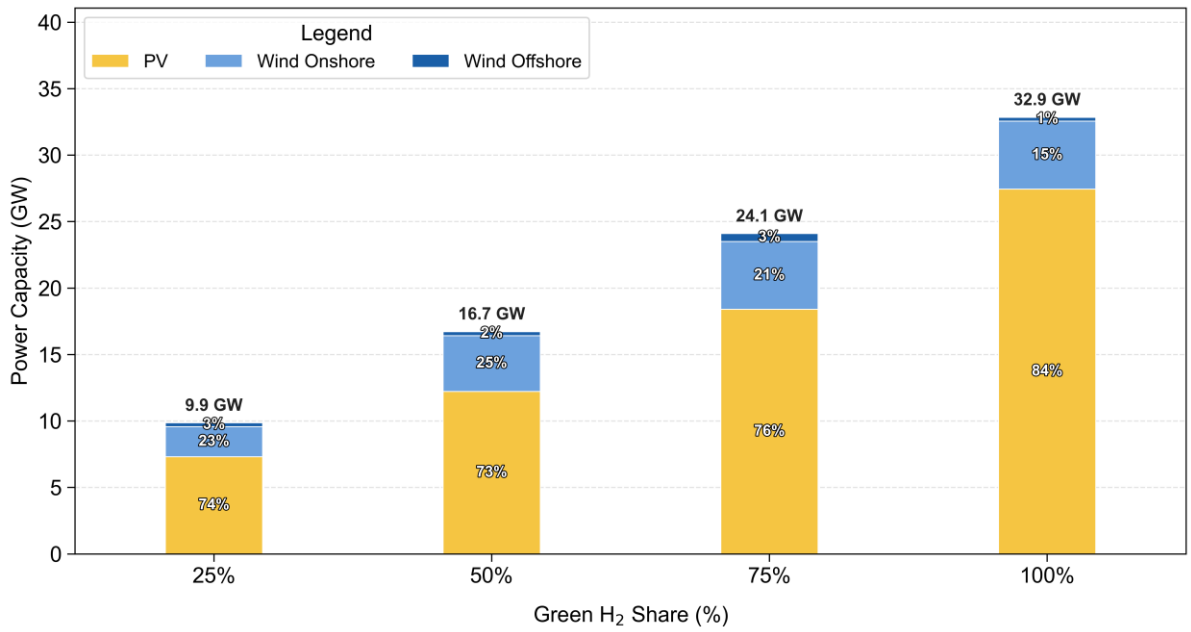


Figure 30. Optimal RES mix for Hybrid-25, Hybrid-50, Hybrid-75 and Green base-case scenarios



Figure 5 shows that LCOH increases with the green hydrogen share. SMR achieves the lowest value, 2.7 €/kgH_2, confirming its cost advantage even with carbon tax. Hybrid scenarios show an almost linear LCOH increase from 3.1 to 4.2 €/kgH_2, driven by RES and electrolysis CAPEX. BESS costs remain nearly stable between Hybrid-25 and Hybrid-50, but rise sharply in the Green scenario, together with hydrogen storage needs. Hybrid-50 therefore emerges as a balanced option, with a substantial green share but without the storage cost escalation of the fully renewable case.

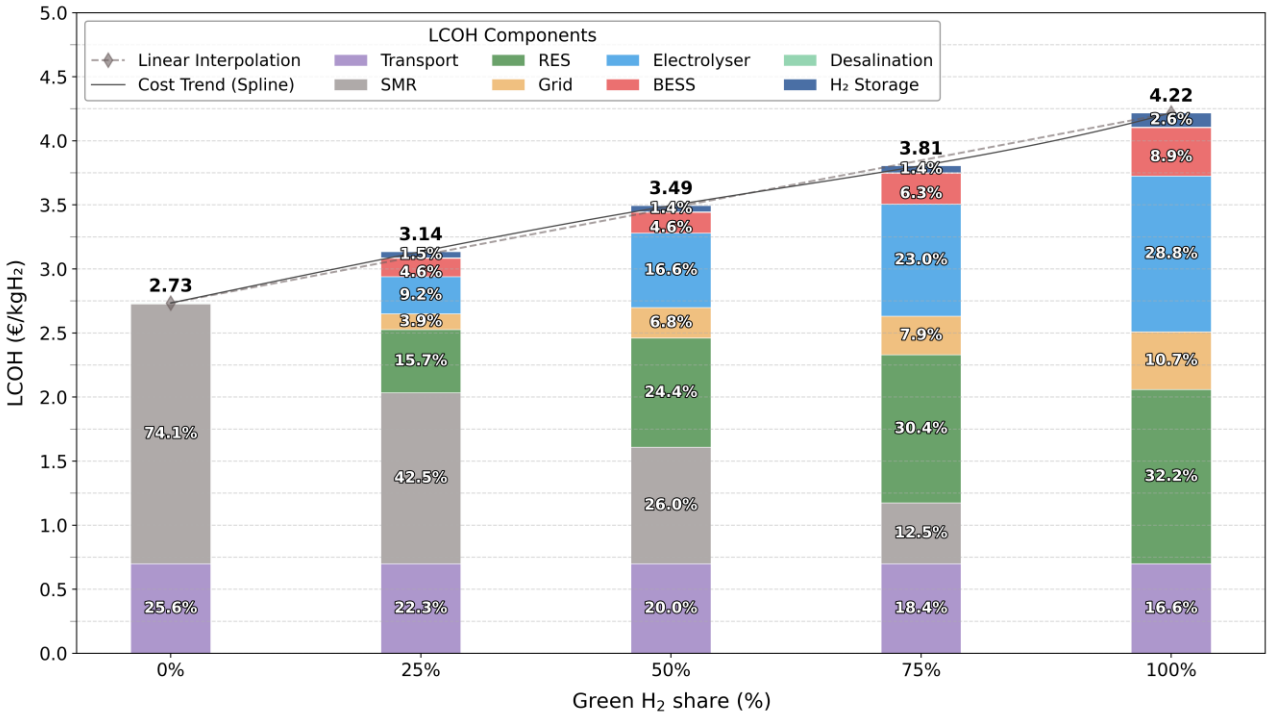


Figure 31. LCOH breakdown for all Base Case scenarios

Figure 6 shows the pressure trends for different sections within the hydrogen distribution network. Results shows that the distributed configuration significantly outperforms the centralized one. In the centralized model, the variable user demand causes rapid pressure fluctuations within the main buffer, forcing frequent and inefficient compressor restarts. By introducing secondary buffers, the system behavior is stabilized, generally requiring only a single daily recharge cycle for civil and mobility users. This fluid-dynamic decoupling leads to a drastic reduction in the overall energy consumed by compression stages, dropping from 900 kWh to roughly 100 kWh.

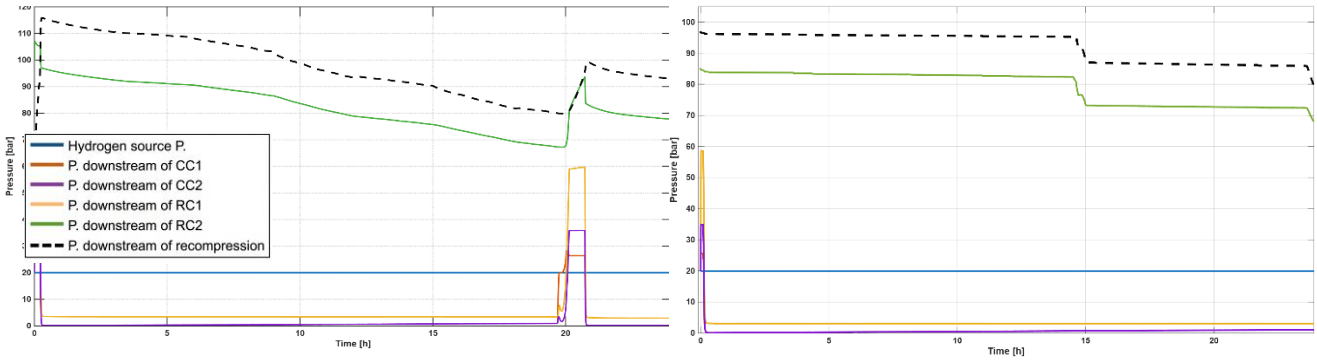


Figure 6. LCOH breakdown for all Base Case scenarios



4. Conclusions

This study assessed a cross-Mediterranean hydrogen supply chain from North Africa to Europe for a demand of 1.35 MtH_2/year, comparing blue, green and hybrid configurations through RES siting, dynamic pipeline modelling and MILP optimization. Results show a RES mix dominated by PV, supported by onshore wind to reduce night-time mismatch, while offshore wind remains marginal. Economically, Blue H_2 gives the lowest LCOH, 2.73 €/kgH_2, whereas Green H_2 reaches 4.22 €/kgH_2 due to higher RES, electrolysis and storage costs.

Dynamic simulations of hydrogen distribution highlight that a distributed network architecture including secondary buffers is highly effective at decoupling transport from end-user demand fluctuations. This approach minimizes mechanical stress on the components and provides a drastic reduction in compression energy consumption.

Acknowledgements

The authors acknowledge financial support by the Italian Ministry of University and Research (MUR) as part of the European Union program NextGenerationEU, PNRR - M4C2 - ECS_00000024 “Rome Technopole”.

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Ni ALLOY NANOWIRE ELECTRODES INTEGRATED IN A ZERO-GAP ALKALINE WATER ELECTROLYZER - (C175)

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Keywords: alkaline water electrolysis, zero-gap cell, nickel alloys, nanowires, hydrogen production

1. Introduction

Alkaline water electrolysis is a promising technology for green hydrogen production, especially when coupled with renewable electricity. However, lowering cell voltage under low-temperature operation requires both efficient non-noble electrocatalysts and optimized cell architectures. Nickel alloys are attractive for alkaline water splitting due to their low cost, tunable composition, and catalytic activity. In this work, nickel alloy nanowire electrodes were integrated into a laboratory-scale zero-gap alkaline electrolyzer to increase the active surface area and overall cell performance. In addition, the life-cycle energy demand and environmental impact of fabricating nanowire electrodes were assessed to identify critical hotspots and provide insights for reducing the environmental footprint of hydrogen production technologies at the laboratory scale.

2. Materials and Methods

Ni alloy nanowires were prepared by template-assisted electrodeposition and tested in a 4 cm^2 zero-gap alkaline water electrolyzer equipped with a Zirfon separator and recirculated KOH electrolyte. The cell architecture was optimized to improve current collection, gas/liquid transport and contact at the separator–electrode interface. Electrochemical performance was evaluated by polarization curves, galvanostatic operation at selected current densities and preliminary stress tests based on current cycling and repeated on/off protocols.

3. Results and Discussion

The optimization of the zero-gap configuration significantly affected the electrochemical response of the cell, confirming that the integration strategy of nanostructured electrodes is as important as the intrinsic catalytic activity of the material. Compared with different configurations based on Ni-pure electrodes with different shapes, the optimized architecture reduced the operating voltage and improved the reproducibility of the cell response under alkaline conditions, reaching approximately 1.67 V at 10 mA cm^{-2} and 1.90 V at 100 mA cm^{-2}.

Using Ni alloy nanowires, the full-cell configuration further improved performance, reaching approximately 1.63 V at 10 mA cm^{-2} and 1.75 V at 100 mA cm^{-2}. This behavior is attributed to the combined effect of the optimized zero-gap cell and the high-surface-area of the nanowire, which increases the number of accessible electroactive sites, as well as the synergistic interaction among the different elements of the electrocatalyst.

Preliminary current-cycling and on/off tests indicated that the optimized zero-gap platform can operate under variable input conditions, suggesting its potential for coupling with intermittent renewable energy sources.



Configuration	V@10 mA cm^{-2}	V@100 mA cm^{-2}	Key finding
Reference Ni zero-gap configuration	**~1.84**	**~2.08**	Stable reference behaviour
Optimized Ni zero-gap architecture	**~1.67**	**~1.90**	Improved interfacial contact and lower cell voltage
Ni alloy NW electrodes on optimized zero-gap architecture	**~1.63**	**~1.75**	Best full-cell performance

Table. Electrochemical performance of selected Ni-based zero-gap configurations and Ni alloy nanowire electrodes.

4. Conclusions

A zero-gap alkaline electrolyzer was developed and integrated with Ni-based alloy nanowire electrodes. The results show that combining an optimized cell architecture with high-surface-area Ni alloy nanowires is an effective strategy to reduce the operating voltage of alkaline water electrolysis. The improved performance and preliminary response under intermittent operation highlight the potential of this approach for efficient and low-cost hydrogen production from renewable electricity.

Acknowledgements

This work was partially financed by the project PUSH2Green (RSH2A_000019, Italian Ministry of Environment and Energy Security – MASE), within the National Recovery and Resilience Plan (PNRR), Mission 2 “Green Revolution and Ecological Transition”, Component 2 “Renewable Energy, Hydrogen, Network and Sustainable Mobility”, Investment 3.5 “Hydrogen Research and Development”, European Union – NextGenerationEU.

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METHANE CHEMICAL LOOPING OVER NI-BASED OXYGEN CARRIERS FOR SUSTAINABLE HYDROGEN PRODUCTION - (C176)

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Keywords: hydrogen production, chemical looping reforming, methane, Ni-based oxygen carriers, CO_2 utilization

1. Introduction

The increasing demand for low-carbon hydrogen is driving the development of methane conversion processes capable of lowering the environmental impact of conventional reforming technologies. In this context, Chemical Looping Reforming (CLR) represents an effective and attractive route because methane activation and catalyst regeneration are separated into cyclic redox steps, enabling hydrogen production and, when CO_2 is used as oxidant, carbon recycling [1]. In this work, Ni-based oxygen carriers were screened for CH_4 chemical looping reforming, alternating methane decomposition with oxidation in air or CO_2. The aim was to correlate hydrogen productivity, carbon formation and cyclic stability with the redox properties and chemical environment of Ni in different oxide matrices [2,3].

2. Materials and Methods

Different Ni-based materials were investigated, in particular Ni-CeO_2 prepared by coprecipitation, Ni/CeO_2 prepared by impregnation, NiMgAl and NiCaAl mixed oxides derived from hydrotalcite-like precursors, and $LaNi_{0.8}Co_{0.2}O_3$ perovskite. Their structural, textural and redox properties were assessed by XRD, BET, H_2-TPR, CH_4-TPR and TG/TPO, and correlated with chemical looping tests based on repeated CH_4 steps alternated with air or CO_2 oxidation, monitoring H_2, CO, CO_2 and carbon removal.

3. Results and Discussion

All investigated oxygen carriers promoted H_2 formation during the CH_4 fuel step, confirming the suitability of Ni-based oxides for chemical looping methane reforming. However, the catalytic behaviour strongly depended on the Ni environment and on the oxidizing atmosphere used during regeneration. CH_4-TPR analyses revealed differences in methane activation among the investigated materials, reflecting the influence of the support composition and metal–support interactions on hydrogen production and redox behaviour.

Carbon formation was also material-dependent. The lowest carbon accumulation was observed for the $LaNi_{0.8}Co_{0.2}O_3$ perovskite, whereas the ceria-based samples showed intermediate carbon deposition. Higher carbon formation was measured for the hydrotalcite-derived NiMgAl and NiCaAl systems. These trends indicate that more active methane decomposition is not necessarily associated with lower carbon accumulation, and that the balance between Ni accessibility, metal-support interaction and oxygen mobility is crucial.

During cyclic operation, all catalysts maintained hydrogen production over repeated redox cycles, but stability depended on whether air or CO_2 was used in the oxidation step. Air efficiently restored the oxidized state and removed deposited carbon, whereas CO_2



allowed carbon gasification while valorizing CO_2 as a mild oxidant. In this latter case, NiCaAl(exHT) showed particularly stable behaviour, while $LaNi_{0.8}Co_{0.2}O_3$ was more sensitive to CO_2 regeneration. Overall, the results demonstrate that optimizing the Ni chemical environment is essential to tune hydrogen productivity, carbon management and regeneration efficiency.

4. Conclusions

Ni-based oxygen carriers are effective materials for hydrogen production through CH_4 chemical looping reforming. The best performance results from a compromise between methane activation, controlled carbon formation and efficient catalyst regeneration. CO_2 regeneration is especially attractive because it couples hydrogen production with carbon removal and CO_2 utilization, supporting the development of circular and low-carbon reforming routes.

Acknowledgements

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EFFECT OF BALANCE-OF-PLANT DESIGN PARAMETERS ON THE LOAD-DEPENDENT SPECIFIC ENERGY CONSUMPTION OF PEM WATER ELECTROLYZER - (C178)

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Keywords: PEM water electrolysis, specific energy consumption, balance-of-plant

1. Introduction

Proton exchange membrane (PEM) water electrolyzers are a promising route to produce hydrogen as a clean fuel, yet most techno-economic studies treat the unit as a single stack with a fixed efficiency and ignore how the balance of plant (BoP) behaves under load [1]. Each BoP component influences total energy consumption in different directions, so their combined share of specific energy consumption (SEC) varies considerably across the operating range, particularly at part load [2]. This work builds on a component-level model and investigates the design parameters of three key BoP components, the hydrogen compressor, the chiller, and the pressure swing adsorption (PSA) dryer, reshaping the load-dependent SEC profile.

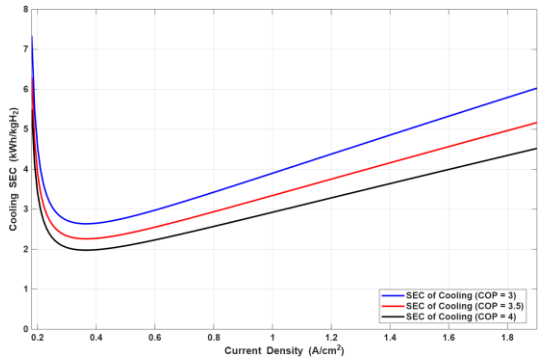
2. Materials and Methods

A steady-state, industrial-scale PEM electrolyzer model at the component level was developed in MATLAB/Simulink. The effects of hydrogen compressor discharge pressure, chiller coefficient of performance (COP), and PEM cathode pressure on the system's total SEC were investigated. For each parameter set, the SEC was solved across the entire operating range (approximately 0.2 to 1.9 A/cm²), and the resulting profiles were compared.

3. Results and Discussion

The results are presented in Fig. 1, where Fig. 1a represents the computed SEC profiles over the full operating range. Fig. 1a shows the system SEC at cathode pressures of 30, 60, and 90 bar, while Fig. 1b shows the cooling SEC for chiller COP values of 3, 3.5, and 4.

a)



b)

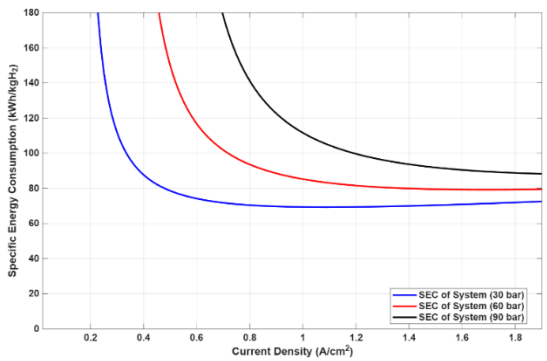


Fig. 1. (a) Effect of the chiller COP (3, 3.5, and 4) on the cooling SEC profile, and (b) Effect of the system delivery pressure (30, 60, and 90 bar) on the system SEC profile,



Increasing the cathode pressure shifts the overall system SEC curve upward, from about 70 kWh/kgH_2 at 30 bar to roughly 80 and 88 kWh/kgH_2 at 60 and 90 bar at nominal load, because the increased PSA dryer purge gas fraction results in a load-independent hydrogen loss. The compressor SEC, set by the pressure-ratio-dependent polytropic work rather than by throughput, rises with discharge pressure from 1.12 kWh/kgH_2 at 200 bar to 1.71 kWh/kgH_2 at 400 bar and 2.11 kWh/kgH_2 at 600 bar, respectively. Fig. 1 shows that increasing the chiller COP from 3 to 4 lowers the cooling SEC by about 25%. SEC falls from 6–7 kWh/kgH_2 near 0.2 A/cm² to a minimum of 2–2.6 kWh/kgH_2 around 0.35–0.4 A/cm², then rises again as the heat load increases. With the PSA purge loss essentially fixed, the dryer dominates at low current density, driving the steep rise below 0.6 A/cm².

4. Conclusions

Varying the compressor, chiller, and PSA dryer parameters reveals three distinct roles in the SEC profile. The SEC value of a compressor is essentially load-independent because the polytropic compression work per unit mass depends on the pressure ratio rather than the flow rate. As the discharge pressure increases, the SEC value of the compressor increases as well. The SEC profile of the chiller depends on the electrolyzer load. As the COP value increases, the average SEC decreases. Increasing the cathode pressure increases the purge gas ratio of the PSA dryer. Therefore, the overall SEC value of the system increases significantly as the load increases. Due to the operating principle of the PSA dryer, the purge gas is constant regardless of the load. Therefore, as the load decreases, the SEC value from the PSA unit increases rapidly. Future work will feed these profiles into a multi-stack techno-economic framework to increase the hydrogen production efficiency.

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ERA JOINT PROGRAMME ON ENERGY STORAGE (C182)

Olga Sumińska-Ebersoldt (KIT), Myriam Gil Bardají (KIT)

Abstract: The European Energy Research Alliance (EERA) Joint Programme on Energy Storage (JP ES) coordinates research efforts to develop advanced, flexible storage solutions supporting Europe's transition to a climate-neutral energy system. Its activities span electrochemical, thermal, mechanical, electrical and chemical storage, with strong emphasis on system integration, sustainability, and sector coupling. A key focus of the programme is the advancement of hybrid energy storage systems (HESS), which integrate complementary technologies to improve the flexibility, efficiency, and reliability of renewable-based energy systems, while also offering a more cost-effective and efficient alternative to existing storage solutions. This is supported by key reference documents copublished by JP ES, including the Technology Roadmap for Hybridisation of Energy Storage, the Strategic Research and Innovation Agenda (SRIA), and the open-access book Hybrid Energy Storage: Case Studies for the Energy Transition. In addition, JP ES has played a leading role in initiating and shaping major European initiatives such as the StoRIES project, which provides access to world-class research infrastructures and advances hybrid storage solutions, and RISEnergy, fostering collaboration and innovation within the renewable energy research community. These activities strengthen knowledge exchange and accelerate the deployment of integrated and sustainable energy technologies. Overall, EERA JP ES plays a central role in shaping research, innovation, and strategic guidance to enable resilient, low-carbon energy systems in Europe, and is actively open to new members to further expand collaboration and impact across the European energy research landscape.

Keywords: energy storage, EERA, hybridisation, HESS, StoRIES, RISEnergy, system integration

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BALTICSEAH$_2$: DEMONSTRATING HYDROGEN ECONOMY WITH THE LARGEST CROSS-BORDER HYDROGEN VALLEY IN EUROPE, BUILDING UP THE VISION - (C185)

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Keywords: hydrogen, hydrogen valley, energy transition, social acceptance, vision

1. Introduction

Hydrogen is increasingly recognized as a key enabler of climate-neutral energy systems, with the potential to decarbonize hard-to-abate sectors such as industry, transport, and energy storage. However, the transition to a green hydrogen economy remains at an early stage and faces challenges related to technology scalability, infrastructure development, economic viability, regulation, environmental sustainability, and social acceptance1. In response, large-scale initiatives such as BalticSeaH2 are promoting cross-border hydrogen value chains and regional hydrogen valleys across the Baltic Sea Region2. This work focuses on developing and analyzing stakeholder-driven visions of a future hydrogen economy within that context. Its novelty lies in integrating technological, economic, environmental, and societal perspectives into shared long-term futures. The visions highlight alternative transition pathways shaped by policy choices, market dynamics, innovation, and public acceptance, providing a foundation for scenario development, strategic planning, and resilient hydrogen transition strategies in the Baltic Sea Region and beyond.

2. Materials and Methods

The study applied a multi-stakeholder co-creation and backcasting framework grounded in sociotechnical transition theory and the Multi-Level Perspective. National workshops (in Finland, Estonia, Sweden, Norway, Denmark, and Poland) engaged stakeholders from the quintuple helix to explore future hydrogen pathways, identify priorities, and co-create national visions via Lego play methodology3. Workshop outputs were qualitatively analyzed and synthesized through a desk-based process into national vision narratives, which were subsequently validated with national partners. The analysis focused on technical, economic, environmental, social, and policy dimensions.

Country	Core Vision	Energy & Infrastructure	Economy & Industry	Society & Governance	Innovation & Strategy
Finland	Hydrogen welfare state balancing society & nature	Diversified renewable electricity; strong national & EU-connected infrastructure	Export of value-added products; attract full hydrogen value chains	Strong local engagement, welfare funding, environmental protection	Strong education system; innovation leadership; risk of low domestic value capture
Estonia	People-driven, innovation-focused small nation	Smart regional hubs; ports & pipelines; wind/solar expansion	Focused value chain choices; potential exporter, importer or tech provider	Local involvement & benefit-sharing; energy security emphasis	Startup-driven innovation; strategic prioritization; testbed potential
Norway	Policy-led transition with local-global balance	Grid upgrades; strategic infrastructure planning; long timelines	Balance domestic value creation with exports; strong supply chains	Strong political leadership; safety, standards, public trust	Builds on oil & gas expertise; CCS potential; workforce transition
Denmark	Hydrogen as means to energy transition	Offshore production; storage (salt caverns); EU-integrated infrastructure & markets	Resource-efficient investments; market-building for hydrogen trade	Public support via policy, incentives, fair benefit-sharing	Export of system-integration knowledge; focus on high-impact uses
Sweden	Integrated system for fossil-free industrial leadership	Highly integrated electricity-hydrogen-heat system; cluster-based infrastructure	Transformation of heavy industry (steel, chemicals); e-fuels from biomass	Strong societal consensus; fairness & shared responsibility	First-mover projects; risk-sharing financing; long-term system coordination
Poland	Pragmatic industrial decarbonization	Integration into industrial hubs; use of district heating; growing renewables	Replacement of fossil hydrogen; hydrogen buses, ports, mobility	Focus on energy security, air quality, workforce reskilling	Flexible, tech-neutral approach; hydrogen valleys development

Table 1. Main results of the visions in the countries (Finland, Estonia, Sweden, Norway, Denmark, and Poland)



Main identified risks
Risk of becoming only a raw hydrogen/energy exporter; local opposition to infrastructure
Limited scale; risk of becoming transit country; dependency on external demand
Slow infrastructure development; dependency on political will; balancing nature vs energy
Dependence on EU demand (especially Germany); resource allocation trade-offs
High dependence on electricity prices; uncertainty around biomass/CO_2 availability
Potential misalignment with EU policies; slower shift from fossil legacy; workforce transition risks

Table 2. Main risks

4. Conclusions

The visions process produced shared national Hydrogen Valley visions for six BSR countries, highlighting common priorities: renewable energy, infrastructure, local benefits, education, innovation, and strategic specialization. The findings show that hydrogen transition pathways will vary across countries and depend on policy, markets, technology, and societal acceptance. Future work will refine the visions through backcasting to identify feasible pathways, actions, trade-offs, and investment priorities for sustainable hydrogen development.

Acknowledgements

The research has been supported by the BalticSeaH2 project (GA ID 101112047), co-funded by the European Union through Clean Hydrogen Partnership call HORIZON-JU-CLEANH2-2022. Authors want to mention also Jatta Jussila & Tiina Laiho (CLIC), Elina Mäki (Gasgrid Finland), Sven Parkel (Estonian Hydrogen Cluster), Vibeke Østlyngen & Knut Linnerud (Energy Valley Norway), Bertil Wahlund (Energiforsk), Cæcilie Haarup

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BEST PRACTICES FOR SCIENTIFIC MANUSCRIPT PREPARATION AND ETHICAL USE OF AI TOOLS - (C179)

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Keywords: scientific publishing, manuscript, research, ethics

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PILOT-SCALE SYNGAS UPGRADING BY TWO-STAGE CATALYTIC TAR CRACKING BASED ON DOLOMITE AND NI/ALUMINA - (C186)

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Keywords: hydrogen, gasification, biomass, catalysis, reforming

1. Introduction

Producing clean hydrogen from lignocellulosic waste is a sustainable route that lowers greenhouse gas emissions and enhances bioeconomy circularity. Two primary conversion pathways exist. The biochemical route (microbial fermentation or enzymatic hydrolysis) is energy-efficient due to lower operating temperatures, but suffers from slower reaction rates, lower yields, and feedstock sensitivity. Conversely, thermo-catalytic processes are fast and continuous, achieving high hydrogen yields despite requiring advanced gas cleaning. Gasification is the dominant thermal method, using sub-stoichiometric oxygen to decompose biomass into syngas (primarily CO, H_2, CO_2, and CH_4). While syngas requires extensive purification to remove condensable organics, catalytic steam reforming of tars further boosts H_2 yields by converting complex molecules. Optimizing industrial production requires developing highly stable, low-temperature catalysts and validating their long-term durability in large-scale, representative systems.

2. Materials and Methods

The study utilized syngas produced by PRAGA gasification plant, which operates with a nominal biomass feed rate of 20 to 30 kg/h [1]. Extracted raw syngas was routed through a thermally insulated pipeline maintained at 250°C to a cracking section housed within a vertical electric furnace. This catalytic section consisted of two tandem reactors connected in series. In the first reactor, dolomite was employed for a dual purpose: it acted as a primary cracking catalyst while simultaneously scavenging sulfur and chlorine impurities. The second stage utilized a nickel-based catalyst supported on alumina. This catalyst was evaluated here for cracking heavier, tar-like organic molecules. The catalytic reforming was tested across a temperature range of 650°C to 750°C and at varying gas hourly space velocities (GHSVs). To continuously monitor non-condensable gas fractions, an online gas chromatography (GC) system was used. Additionally, syngas was sampled at both the gasifier outlet and downstream of the catalytic unit. These samples underwent characterization to quantify water and volatile organic compounds in accordance with the CEN/TS 15439:2006 standard. Ultimately, tar conversion efficiencies and overall hydrogen yields were calculated by combining these analytical results with a nitrogen-based mass balance.

3. Results and Discussion

The experimental investigation demonstrated the high efficiency of a catalytic treatment process for upgrading syngas extracted directly from the gasifier bed. Analysis revealed that syngas streams had higher tar concentrations of around 100 g/m³. The syngas streams contained an excess of water, providing ideal over-stoichiometric conditions for steam reforming. The subsequent catalytic treatment, utilizing a dolomite pre-stage and a Ni-based catalyst, achieved remarkable tar conversion efficiencies exceeding 98.5%, significantly outperforming comparable literature benchmarks. This treatment resulted in a substantial upgrade of the syngas. Hydrogen content increased on average from 21vol% in the raw syngas to 31vol% in the reformed stream. This new hydrogen was primarily generated through the steam reforming of tar, supplemented by the Water-Gas Shift (WGS) reaction converting CO into H_2. The process also expanded the total gas volume. The dolomite played a crucial multifaceted role, acting as a contaminant trap,

aiding in tar reforming. Ultimately, the comprehensive reforming process led to a significant energy gain, enhancing the Lower Heating Value (LHV) of the treated syngas [2].



Figure 1: The gasification plant PRAGA (up draft gasification) and the section of tar steam reforming on the right at ENEA CR of Trisaia.

4. Conclusions

In this study, we demonstrated a highly effective approach for biomass tar conversion via catalytic steam reforming at the pilot scale. This system confirmed a distinct increase in real tar abatement capacity, achieving remarkable conversion rates of 98.5–99.5%. Concurrently, the treatment significantly upgraded the upstream syngas. The H_2 content increased by concentration and in molar terms. This success relies on a dual-reactor strategy that couples two catalysts: one cheap and moderately performant, and another that is more expensive and complex to produce.

Acknowledgements

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NEW COMPOSITE ADSORBENTS FOR THERMOCHEMICAL HEAT STORAGE - (C193)

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Keywords: up to five keywords separated by commas.

1. Introduction

The aim of this work is the preparation and characterization of novel composite adsorbents based on 1-ethyl-3-methylimidazolium acetate (EMIM-Ac), a room-temperature ionic liquid known for its strong hydrophilic nature [1, 2], supported on mesoporous silica gel for thermochemical heat storage at low temperature (T < 100 °C). The resulting silica/[EMIM-Ac] composite demonstrated a superior water sorption capacity (up to 0.71 g/g at 80% RH for a 50 wt% IL loading) compared to other state-of-the-art adsorbents [3]. Full process reversibility and negligible adsorption/desorption hysteresis were also verified, together with thermal stability up to approximately 220 °C, as confirmed by TGA analysis. These features are particularly important for practical operation in thermochemical heat storage systems. The structural stability of samples subjected to repeated adsorption/desorption aging cycles was assessed by FT-IR, high-resolution solid-state NMR, and time-domain NMR spectroscopy. Finally, a simplified thermodynamic analysis based on the experimental adsorption data indicates that the silica/[EMIM-Ac] composite is highly suitable for adsorption heat storage, providing a volumetric energy density of 600–920 MJ/m^3. This performance is very promising for the design of compact and efficient thermochemical heat storage systems driven by low-temperature heat sources.

2. Results and Discussion

The resulting silica/[EMIM-Ac] composite demonstrated a superior water sorption capacity (up to 0.71 g/g at 80% RH for a 50 wt% IL loading) compared to other state-of-the-art adsorbents [3]. Full process reversibility and negligible adsorption/desorption hysteresis were also verified, together with thermal stability up to approximately 220 °C, as confirmed by TGA analysis. These features are particularly important for practical operation in thermochemical heat storage systems. The structural stability of samples subjected to repeated adsorption/desorption aging cycles was assessed by FT-IR, high-resolution solid-state NMR, and time-domain NMR spectroscopy. Finally, a simplified thermodynamic analysis based on the experimental adsorption data indicates that the silica/[EMIM-Ac] composite is highly suitable for adsorption heat storage, providing a volumetric energy density of 600–920 MJ/m^3. This performance is very promising for the design of compact and efficient thermochemical heat storage systems driven by low-temperature heat sources.

Acknowledgements

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ENERGY STORAGE INNOVATION IN ITALY: BATTERY TECHNOLOGY EVOLUTION AND THE "RICERCA DI SISTEMA" PROGRAMME – (C194)

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1. Introduction

The transition towards climate-neutral energy systems has placed energy storage among the highest priorities of European research and innovation. Energy storage is increasingly recognized as a key enabling technology for the large-scale deployment of renewable energy sources, ensuring grid flexibility, reliability and resilience while supporting the achievement of the European decarbonization targets for 2050. Within this framework, considerable efforts are being devoted to the development of sustainable, efficient and economically competitive storage technologies, with particular emphasis on advanced materials, circular manufacturing strategies and nextgeneration electrochemical systems.

2. Results and Discussion

In recent years, the battery concept has evolved from an end-of-life perspective to a life-cycle-based approach, where batteries are managed as traceable digital assets throughout their entire value chain, in compliance with the European Battery Regulation (EU) 2023/1542 (Fig. 1). Consistent with European policies and the objectives of the Italian National Integrated Energy and Climate Plan (PNIEC), Italy has launched a coordinated national research strategy through the Ricerca di Sistema Elettrico (RdS) programme, which promotes innovation in strategic energy technologies. Within this framework, the Italian National Research Council (CNR), ENEA and RSE have jointly developed research activities aimed at advancing both electrochemical and thermal energy storage solutions.

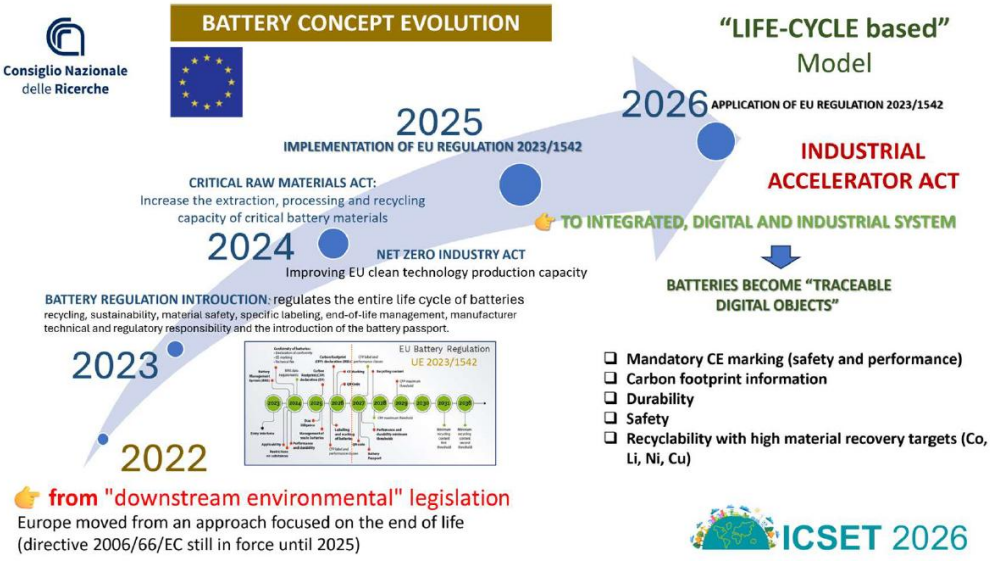


Fig.1 Battery concept evolution in EU



This contribution introduces the objectives of the new PTR 25–27 Integrated Project, which further expands these activities through the development of innovative storage concepts, advanced materials and next-generation electrochemical and thermal technologies. Finally, the main findings and key conclusions of the ORANGEES project, completed in May 2026, will be presented, providing an overview of the project's most relevant scientific and technological achievements and their impact on the future development of sustainable energy storage technologies.

Acknowledgements

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POLISHING METHANE-CONTAINING GAS STREAMS TO NATURAL GAS GRID SPECIFICATIONS USING ALUMINA-CARBON MOLECULAR SIEVE MEMBRANES - (C196)

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Keywords: Carbon membranes, Gas separation, H_2 Deblending, Power to Methane, CO_2 utilization.

1. Introduction

The increasing deployment of renewable energy sources requires efficient energy storage solutions to manage surplus electricity and support grid stability. In this context, hydrogen is attracting growing interest as an energy carrier, as surplus renewable electricity can be converted into green H_2 via electrolysis. However, hydrogen storage and distribution remain challenging. One option is blending H_2 into the natural gas grid and separating it before end use. Alternatively, hydrogen can be converted into synthetic natural gas (SNG) through Power-to-Methane (PtM), enabling storage and transport using existing infrastructure. The EU-funded MEASURED project investigates alumina–carbon molecular sieve membranes (Al-CMSMs) for both hydrogen deblending and methane polishing applications. Similar Al-CMSMs have previously been reported as promising candidates for the separation of low hydrogen concentrations (5–20 vol%) from H_2/CH_4 mixtures, achieving a hydrogen purity of 99.4% in the permeate when processing feed streams containing 10 vol% H_2 [1]. This work presents Al-CMSMs incorporating boehmite nanoparticles for hydrogen deblending and PtM applications, with particular emphasis on obtaining a methane-rich retentate stream that complies with natural gas grid specifications.

2. Materials and Methods

Alumina-carbon molecular sieve membranes were prepared on asymmetric tubular alumina supports by a one dip-dry-carbonization method [2]. The supports were coated with a solution containing Novolac phenolic resin, formaldehyde, ethylenediamine, boehmite nanoparticles and N-methyl-2-pyrrolidone (NMP), followed by drying at 95°C overnight. The coated supports were subsequently carbonized at 550°C for 2 h under controlled heating conditions (1°C min^{-1}) to obtain the final carbon selective layer. The resulting Al-CMSMs were characterized through single-gas and mixed-gas permeation tests both with CH_4-H_2 binary mixtures and ternary CO_2-CH_4-H_2 mixtures.

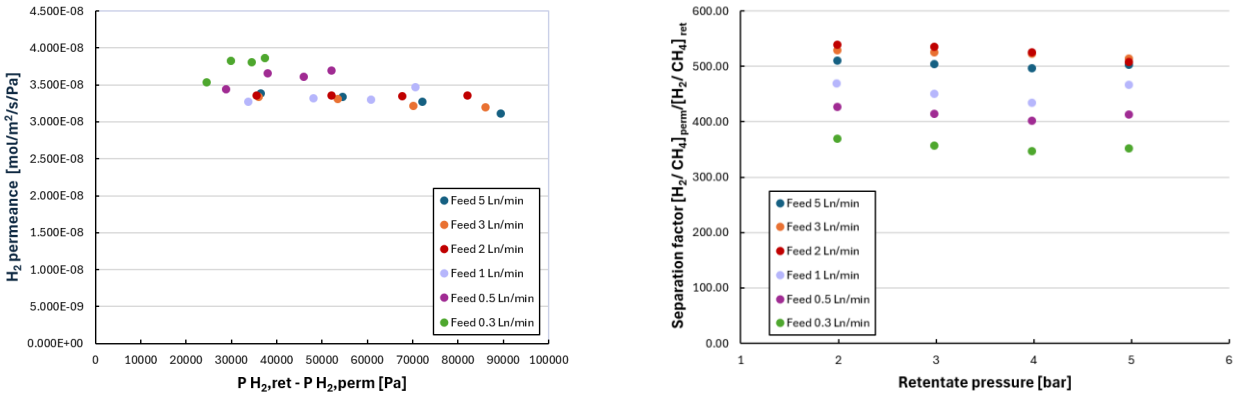
3. Results and Discussion

The single gas permeation tests were performed with humified membranes and after the activation of the membranes at different temperatures ranging from 60°C to 150°C. The results show that the permeance depends on the kinetic diameter of the permeating gas and the temperature of permeation, as well as the presence of humidity in the pores of the membranes.

The membranes display hydrophilic behavior, molecular sieving and surface diffusion transport mechanisms are observed. The presence of adsorbed water in the pores enhances CO_2 permeation via surface diffusion mechanism, thereby improving H_2/CO_2 selectivity. At higher membranes activation temperatures, the removal of water from the pore structure reduces this contribution, resulting in lower H_2/CO_2 selectivity.



Figure *1a* and *1b* report the mix-gas permeation test results in case of a binary CH_4-H_2 mixture with 20% vol. H_2 at 30°C, with vacuum permeate and a retentate pressure ranging from 2 to 5 bar.



(a) (b)

Figure 32: Mix gas permeation tests at 30°C using binary CH_4-H_2 mixture with 20% vol. H_2 at 30°C, with vacuum permeate and a retentate pressure ranging from 2 to 5 bar. H_2 permeance trends with respect to partial pressure difference at different feed flowrates (a) and separation factor trends with retentate pressure (b).

Looking at the mix-feed tests, the methane rejection indicates that methane is preferentially retained on the retentate side of the membrane, as indicated by the high methane rejection Higher permeances are achieved at lower feed flow rates, resulting in a slight decrease in both the H_2/CH_4 separation factor and methane rejection, while enhancing hydrogen recovery.

4. Conclusions

The permeation results show that the permeance depends on the kinetic diameter of the permeating gas and the temperature of permeation, as well as the presence of humidity in the pores of the membranes. Additionally, they suggest that the Al-CMSM could be used for the CH_4 polishing in the CO_2 methanation process and for the hydrogen deblending applications.

Acknowledgements

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EUROPEAN VISION AND STRATEGIC RESEARCH AND INNOVATION AGENDA FOR THE BATTERY SECTOR: STATE OF PLAY AND FUTURE ACTIONS OF THE SET PLAN IMPLEMENTATION WORKING GROUP - (C197)

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Keywords: SET-Plan, Batteries, Europe strategy, SRIA, IWG.

The rapid deployment of sustainable and competitive battery technologies is essential to achieving Europe's climate neutrality objectives while strengthening energy security, industrial competitiveness, and technological sovereignty. As batteries become a strategic pillar of the clean energy transition, coordinated research and innovation actions are increasingly needed to accelerate technological progress, reinforce the European value chain, and reduce dependencies on critical raw materials and non-European manufacturing capacities.

Within this context, the European Strategic Energy Technology (SET) Plan plays a central role in aligning national and European research priorities. This presentation provides an overview of the ongoing activities of the SET Plan Implementation Working Group (IWG) on Batteries, with particular focus on the development of the renewed European Vision and Strategic Research and Innovation Agenda (SRIA). Building upon the achievements of previous SET Plan initiatives, the updated strategic framework responds to emerging technological, industrial and geopolitical challenges by adopting a broader systems perspective that encompasses advanced battery chemistries, sustainable materials, circularity, manufacturing innovation, digitalisation, safety, recycling, and integration across multiple application sectors.

The presentation will illustrate the methodology adopted to define the new strategic priorities and long-term objectives for 2030, 2040 and 2050, highlighting the collaborative process involving Member States, research organisations, industry, and European partnerships. The renewed SRIA is designed to strengthen synergies between national programmes and European initiatives, supporting the implementation of the Clean Industrial Deal, the Competitiveness Compass, and the evolving European policy framework for clean technologies.

Finally, the contribution will discuss the next steps towards the completion and implementation of the updated strategic documents, identifying opportunities for stakeholder engagement and international cooperation to accelerate the deployment of safe, sustainable and globally competitive battery technologies, thereby reinforcing Europe's resilience and leadership in the energy transition.

Acknowledgements

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LOW-TRANSITION-TEMPERATURE ELECTROLYTES FOR RECHARGEABLE ZINC BATTERIES - (C199)

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Keywords: deep eutectic electrolytes, zinc metal anodes, rechargeable batteries.

1. Introduction

Zinc-ion batteries (ZIBs) using aqueous electrolytes still face critical issues: dendrite formation, hydrogen evolution from water splitting, and zinc corrosion or passivation due to side reactions [1]. To mitigate these challenges, replacing aqueous electrolytes with low-transition-temperature (LTT) mixtures has been proposed. LTT mixtures offer the benefits of low volatility and flammability, ensuring safety, along with simple preparation and environmental friendliness [2]. Furthermore, addressing dendrite growth on zinc metal anodes requires forming a stable anion-based solid electrolyte interphase (SEI). This can be achieved by using fluorine-containing salts like zinc-bis(trifluoromethanesulfonyl)imide, $Zn(TFSI)_2$, whose $TFSI^-$ anion aids in creating a F-rich SEI [3].

2. Materials and Methods

Novel LTT mixtures, based on $Zn(TFSI)_2$ and ethylene glycol (EG) at various molar ratios, were prepared and characterized using thermal and spectroscopic techniques to understand molecular interactions and electrochemical methods to assess performance and applicability. Also, hydrated electrolytes based on LiTFSI, $Zn(TFSI)_2$, and urea were investigated for application in Li/Zn dual-ion batteries employing $LiMn_2O_4$ (LMO) cathodes.

3. Results and Discussion

Among the formulations containing EG solvent, the Zn:EG mixture at a 1:7 molar ratio proved to be the most promising for battery applications. This optimized LTT electrolyte was evaluated in a full-cell configuration, pairing a zinc metal anode with a novel K^+-doped vanadium oxide ($K_{0.5}V_2O_5$, KVO) cathode.

With respect the dual ion compositions, different amounts of ultrapure water were incorporated into the LTT mixture in order to optimize ionic conductivity while preserving the intrinsic eutectic network and electrochemical stability. Differential scanning calorimetry confirmed the successful preservation of eutectic systems and demonstrated that water molecules are integrated into the hydrogen-bonding network. FT-IR analysis further verified the establishment of intermolecular interactions among the components. Electrochemical impedance spectroscopy showed that increasing water content progressively decreased ohmic resistance and enhanced ionic conductivity, reaching approximately 0.40 mS cm^{-1} for the most hydrated DES formulation (H_2O concentration of 37 mol%). Galvanostatic plating/stripping experiments in Zn||Zn symmetric cells demonstrated that hydrated LTT electrolytes significantly improve zinc deposition reversibility and suppress dendritic growth compared with the anhydrous system.

4. Conclusions

Physical chemical characterizations of the proposed LTT mixtures confirm their applicability as safe electrolytes for battery applications. The electrochemical cell tests demonstrated encouraging performance, suggesting that selected LTT electrolyte effectively supports stable cycling and mitigates dendritic growth. While challenges remain, these findings underscore the potential of LTT mixtures as a viable and eco-friendly electrolyte option for next-generation zinc-ion batteries.



Acknowledgements

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SUSTAINABLE ENERGY STORAGE: ASSESSING INNOVATIVE MATERIALS THROUGH LIFE CYCLE ASSESSMENT – (C200)

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Keywords: Life Cycle Assessment, Energy Storage, Innovative Materials, Environmental Impacts, Eco-design.

1. Introduction

The deployment of renewable energy technologies requires efficient energy storage systems to support the energy transition. While batteries are key enablers of decarbonization, their production depends on critical raw materials and generates significant environmental impacts throughout the life cycle. Therefore, developing innovative materials with lower environmental footprints has become a research priority. Although Life Cycle Assessment (LCA) has been widely applied to commercial battery technologies, fewer studies address emerging materials at the laboratory stage. This work highlights the role of LCA in assessing innovative materials, identifying environmental hotspots, comparing alternative solutions, and supporting eco-design from the early stages of technology development.

2. Materials and Methods

The study describes the application of the LCA methodology according to ISO 14040 and ISO 14044 standards to assess the environmental performance of innovative materials for electrochemical energy storage. Primary laboratory data are integrated with secondary data from internationally recognized databases. Environmental impacts are quantified through midpoint indicators, while contribution analyses are performed to identify lifecycle hotspots and support eco-design strategies.

3. Results and Discussion

The application of LCA to innovative storage materials demonstrates its potential to guide the development of more sustainable energy storage technologies beyond conventional energy-performance indicators. By integrating environmental aspects into material selection and cell design, LCA enables the comparison of alternative solutions with equivalent electrochemical performance while highlighting differences in resource consumption, greenhouse gas emissions, and other environmental impact categories. The results show that the production of active materials and energy-intensive manufacturing steps often represent the main environmental hotspots. The analysis also highlights the influence of critical raw materials on the overall environmental profile, emphasizing the potential benefits of alternative chemistries based on abundant, renewable, recycled, or bio-based materials. Such information supports the identification of improvement opportunities, including material substitution, process optimization, energy efficiency measures, and enhanced circularity. Furthermore, applying LCA during the early design phase allows potential environmental trade-offs to be identified before industrial scale-up, reducing the risk of transferring technologies associated with higher environmental impacts to the market. LCA can also support the assessment of emerging technologies under future production scenarios, providing valuable guidance for research and innovation activities aimed at sustainable battery development.



4. Conclusions

LCA represents a key methodology for supporting the sustainable development of next-generation energy storage systems. By identifying environmental hotspots and quantifying the potential benefits of innovative materials, LCA provides scientifically sound information for eco-design, technology optimization, and future scale-up. Integrating environmental assessment into research and development contributes to reduce the life-cycle impacts of energy storage technologies while supporting circular economy and decarbonization objectives.

Acknowledgements

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CEETe H_2: AN INTEGRATED PLATFORM FOR HYDROGEN TECHNOLOGIES – (C204)

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Keywords: CEETe H2, hydrogen safety, digital twin, renewable energy, electrolysis

1. Introduction

Hydrogen is expected to become a cornerstone of future low-carbon energy systems, yet the lack of integrated research infrastructures limits the validation of hydrogen technologies under realistic operating conditions. Existing pilot facilities usually focus on individual components rather than the complete hydrogen value chain. The CEETe H_2 project addresses this gap by developing a comprehensive Hydrogen Hub integrating renewable hydrogen production, storage, distribution, refueling, battery storage and advanced digital monitoring within a university campus. The proposed infrastructure enables interdisciplinary research, technology validation, digital twins and predictive control, creating a unique platform for accelerating hydrogen deployment in smart energy systems and sustainable transport.

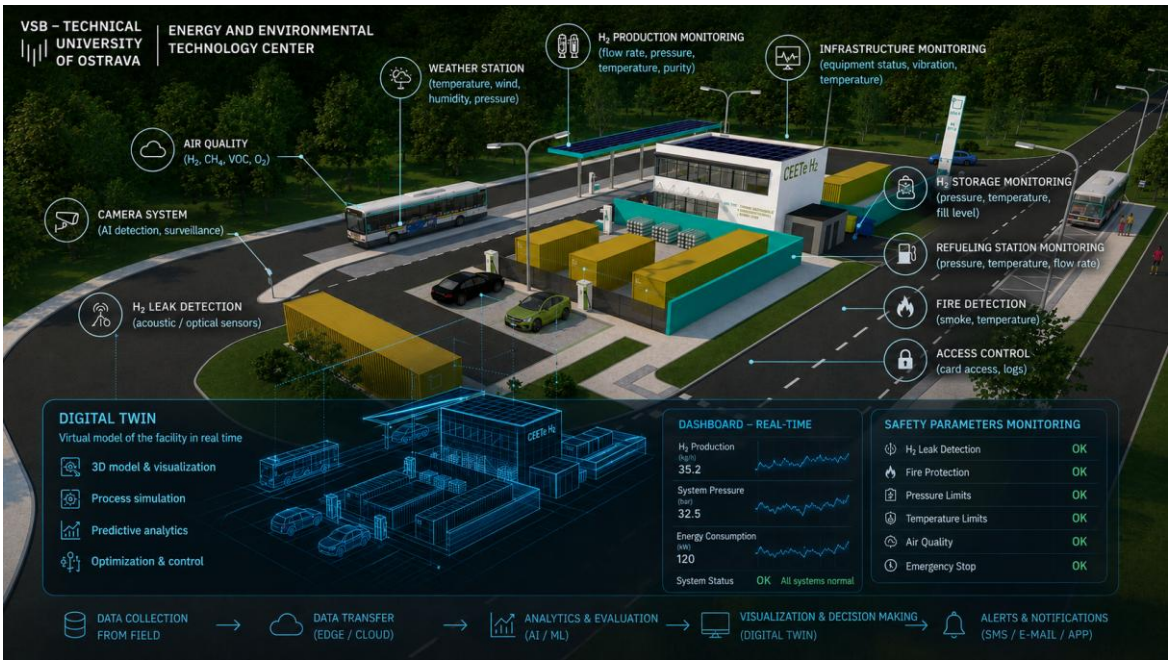


Figure 1. Functional concept of the CEETe H_2 Hydrogen Hub

2. Materials and Methods

The proposed infrastructure combines a 350–400 kW PEM electrolyser (100–150 kg H_2 day^{-1}), 200 kg hydrogen storage, 350/700 bar refuelling station, 2 MW battery storage, SCADA-based energy management and an extensive sensor network. Digital twin



models integrate operational data from electrolysers, compressors, storage tanks and dispensers for performance optimisation, predictive maintenance and safety analysis.

3. Results and Discussion

The CEETe H_2 concept represents an integrated research infrastructure covering the complete hydrogen value chain—from renewable hydrogen production to end-use applications. The platform consists of four specialised laboratories focusing on (i) low-carbon fuel conversion and hydrogen production, (ii) hydrogen and battery energy storage, (iii) hydrogen distribution and refuelling technologies, and (iv) safety monitoring and predictive risk management.

The hydrogen production laboratory is equipped with a 350 kW PEM electrolyser, hydrogen purification, compression up to 900 bar and advanced process monitoring. The storage laboratory combines high-pressure hydrogen vessels (500 and 900 bar) with a 2 MW battery storage system, enabling hybrid energy management and renewable energy integration. Distribution research includes laboratory-scale hydrogen refuelling stations, cooling systems, hydrogen quality monitoring and digital optimisation of refuelling protocols according to European standards. The Safety and Monitoring Laboratory integrates approximately one hundred hydrogen detectors, predictive AI algorithms, emergency simulations, SCADA monitoring and cybersecurity modules to improve operational reliability.

Unlike conventional hydrogen demonstration facilities, CEETe H_2 is designed primarily as an open research platform enabling experimental validation, digital twin development, predictive maintenance, safety assessment and interdisciplinary cooperation. The infrastructure provides experimental data for optimisation of hydrogen production efficiency, storage behaviour, refuelling performance and integrated operation of smart energy systems, supporting future Hydrogen Valleys and low-carbon transport applications.

Table 1. Planned research infrastructure of the CEETe H_2 Hydrogen Hub

Laboratory	Main research focus
Low-Carbon Fuel Conversion & Synthesis	PEM electrolysis, hydrogen production, compression
Energy Storage	Hydrogen storage, battery systems, hybrid energy management
Distribution & Utilisation	Refuelling technologies, pipelines, hydrogen quality
Safety & Monitoring	Leak detection, AI prediction, digital twin, SCADA

4. Conclusions

The CEETe H_2 Hydrogen Hub provides a comprehensive research infrastructure integrating hydrogen production, storage, distribution, utilisation and safety into a single experimental platform. The combination of digital twins, predictive monitoring and smart energy management creates new opportunities for research on Hydrogen Valleys, renewable integration and low-carbon mobility. The infrastructure is expected to accelerate technology validation and support future industrial deployment.



Poster

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HARNESSING LOW-VELOCITY TIDAL CURRENTS: DUCT-OPTIMIZED TURBINES AND DIVER-LESS MAINTENANCE FOR BRIDGE-INTEGRATED POWER – (C002)

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Keywords: tidal current power, low-velocity flow, ducted hydrokinetic turbine, bridge-integrated energy

1. Introduction

Tidal current energy is an attractive renewable resource due to its high energy density, long-term predictability, and limited sensitivity to weather conditions. When integrated into bridge structures, tidal currents and river flows acting on bridge piers can be harnessed to supply local loads such as lighting and monitoring systems, even in low-velocity environments. However, most commercial tidal current turbines require a current speed of about 2 m/s, whereas typical bridge sites exhibit significantly lower velocities. This study therefore focuses on three key technologies to enhance feasibility at such sites: frictionless sealing to reduce mechanical losses and cut-in speed, duct systems to amplify inflow velocity toward the rotor, and a diver-less operation and maintenance concept suitable for devices attached to bridge columns.

2. Materials and Methods

The turbine employs a magnetic coupling-based frictionless sealing system that separates the wet rotor from the dry generator, preventing seawater ingress while minimizing mechanical friction. Three duct geometries—nozzle, diffuser, and nozzle-diffuser combined—are designed with common length and diameter parameters and evaluated using RANS-based CFD with an SST turbulence model. A scaled model matching a circulating water channel facility is used to analyze velocity amplification. For O/M, a rail-and-winch system attached to bridge columns is proposed, enabling vertical retrieval of the turbine module from the bridge deck without divers.

3. Results and Discussion

The CFD analysis reveals distinct pressure and velocity profiles across the examined duct geometries. In the nozzle-type duct, the converging inlet produces a region of elevated stagnation pressure, leading to a limited velocity increase, whereas the diffuser-type duct generates a low-pressure zone near the expanding outlet that promotes smoother and more uniform flow acceleration. The combined nozzle-diffuser configuration integrates both mechanisms, accelerating the inflow and lowering the outlet pressure concurrently, thereby sustaining higher centerline velocities. At an upstream velocity of 1 m/s, this configuration achieves a centerline velocity amplification factor of approximately 1.46, outperforming the individual nozzle and diffuser designs and demonstrating superior suitability for low-velocity tidal environments.

Since power output scales with the cube of flow velocity, this amplification translates into a significant enhancement of potential energy yield, particularly when coupled with a high-torque turbine and a frictionless magnetic sealing system that lowers the operational cut-in speed. Experimental validation in a circulating water channel confirms the numerical findings, exhibiting improved rotor efficiency at low tip-speed ratios for the ducted arrangements. Moreover, the proposed diver-less operation and maintenance system for bridge-integrated turbines—utilizing guide rails and a deck-mounted winch—facilitates module retrieval above the water surface for inspection or component replacement. This approach eliminates diving requirements, reduces



maintenance costs, and enhances operational safety, making it particularly advantageous for small-scale, bridge-based energy installations.

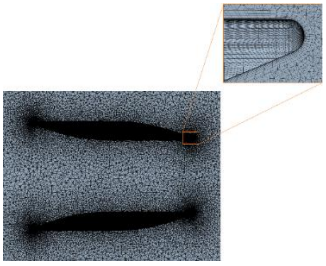


Figure 1. Generating mesh around duct

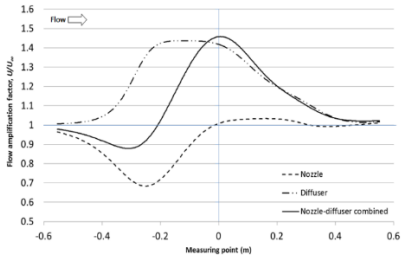


Figure 2. Flow velocity amplification

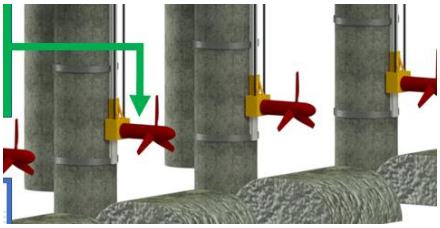


Figure 3. Tidal current system to bridge

4. Conclusions

This study shows that tidal current power can be effectively integrated into bridge structures in low-velocity environments when supported by optimized ducts, frictionless sealing, and a practical O/M strategy. Among the examined geometries, the nozzle-diffuser combined duct provides the highest velocity amplification and is therefore the most suitable for enhancing turbine inflow under weak currents. Together with magnetic coupling-based sealing and a diver-less rail-and-winch maintenance system, this configuration can reduce cut-in speed, simplify field operations, and improve the overall feasibility of bridge-integrated tidal current systems intended for local power supply.

Acknowledgements

The research presented in this study was supported by the KAIA research program "Development of Marine Bridges Operation using Green Energy," funded by the Ministry of Land, Infrastructure and Transport (Grant Number: RS-2024-00401101).

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CATHODE MATERIALS AND ELECTROLYTE FORMULATIONS FOR EMERGING POTASSIUM-SULFUR BATTERIES – (C003)

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Keywords: Potassium-sulfur batteries, Sulfur-hosting cathode, Glyme-based electrolytes, High-concentration electrolyte, Shuttle effect.

1. Introduction

Potassium-sulfur batteries (KSBs) are emerging as a promising energy storage system due to the high natural abundance of the active materials and the high theoretical energy density[1]. This system (with the first room-temperature cell reported in 2014) exploits the same conversion mechanism as lithium-sulfur batteries (LSBs), which involves a two-electron transfer for each sulfur atom responsible for the high theoretical specific capacity of sulfur[2]. Akin to LSBs, KSBs face challenges limiting their practical application, including cathodic volume expansion, sluggish reactions kinetics, shuttle effect, sulfur insulating nature, and potassium dendrite growth[3]. This work explores sulfur-hosting cathodes and compatible electrolytes, aiming at assembling a prototype KSB.

2. Materials and Methods

Electrodes were prepared by melt infusion of sulfur (40 wt%) into carbon materials; the composite was mixed with PVDF binder (10 wt%) and NMP to prepare slurries, which were cast onto aluminum foil. Coin cells were assembled with potassium metal anodes, Whatman glass fiber separators, and electrolytes with various solvents and salts. Electrochemical characterization included galvanostatic cycling (GC) and cyclic voltammetry (CV).

3. Results and Discussion

The study initially employed commercial Ketjenblack EC-300J (KJB) as sulfur host, a benchmark material for lithium sulfur batteries; additional carbon hosts, including CMK-3, YP-50F Kuraray, and Multiwalled carbon nanotubes, were also investigated. Carbonate electrolytes were investigated using a 1:1 vol% ethylene carbonate (EC)/diethyl carbonate (DEC) solvent solution and diverse salts, including potassium bis(fluorosulfonyl)imide (KFSI) and potassium bis(trifluoromethanesulfonyl)imide (KTFSI). GC showed characteristic discharge plateaus and corresponding CV peaks related to sulfur conversion only during the first discharge. Subsequent cycles were dominated by capacitive potassium storage, due to the irreversible consumption of polysulfides through nucleophilic addition or substitution reactions with carbonate solvents. This interpretation was supported by comparison with sulfur-free electrodes, which exhibited similar electrochemical behavior after the first cycle. Ether-based electrolytes were then explored using diethylene glycol dimethyl ether (DEGDME) and tetraethylene glycol dimethyl ether (TEGDME). The most stable system was obtained using KJB as sulfur host, TEGDME with KTFSI (1 M), and a potential window between 1.2 and 2.4 V vs K^+/K, with pronounced sulfur conversion peaks observed in the CV. However, GC tests still evidenced polysulfide shuttling from the first cycle, as prolonged charge process was recorded. Increasing the electrolyte concentration to 2 M effectively mitigated this effect, enabling a stable conversion mechanism for at least 30 cycles, as reported in Figure 2. However, the improved suppression of the polysulfide shuttle is accompanied by an increased irreversible deposition of poorly soluble polysulfide species, which negatively affects the long-term reversibility of the system.



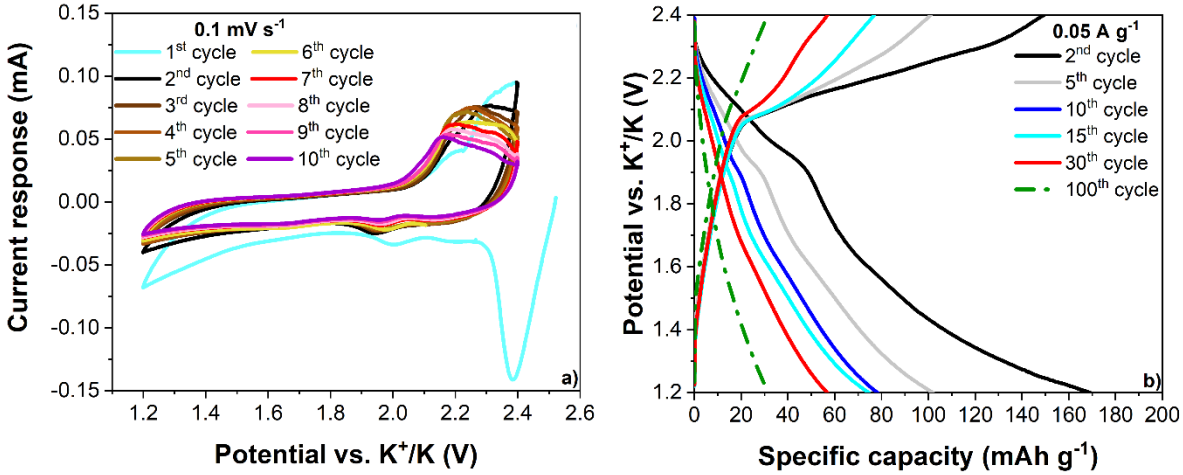


Figure 1. Electrochemical characterization of the cell assembled using KJB as sulfur host and TEGDME, KTFSI (2 M): a) CV and b) galvanostatic profiles.

4. Conclusions

The most relevant results were obtained using KJB as sulfur host and TEGDME with 2 M KTFSI electrolyte, enabling stable conversion for at least 30 cycles and mitigating shuttle effect. Further research is required to optimize slurry and electrolyte formulations, using alternative solvents and exploring the localized high concentration electrolyte strategy. Moreover, the utilization of single-atom catalysts could be essential to improve reaction kinetics and system reversibility.

Acknowledgements

This work was supported by the LOTUS project (Lithium prOtecTion for robUst and Safe batteries), funded by the Ministero dell'Università e della Ricerca (MUR), grant number R20RKNBS7E.

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EFFICIENT MOF-BASED CATALYSTS FOR THE DIRECT SYNTHESIS OF DIMETHYL CARBONATE (DMC) FROM CO_2 AND METHANOL – (C013)

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Keywords: CO_2 valorization, dimethyl carbonate, MOFs-based catalysts, BiPF-7, green chemistry.

1. Introduction

The direct synthesis of dimethyl carbonate (a solvent widely used in organic reactions such as methylation, carbonylation and carboxymethylation) from CO_2 and methanol constitutes an environmentally benign alternative to the conventional phosgene-based route [1]:

$$CO_2 + 2\ CH_3OH \rightleftharpoons \mathbf{(CH_3O)_2CO} + H_2O \qquad (1)$$

However, this process is limited by the high thermodynamic stability of the CO_2 molecule and by an unfavorable reaction equilibrium toward DMC formation. According to thermodynamic considerations, operation at low temperatura and elevated pressure is required, making the use of efficient catalysts essential to enhance the reaction rate [2]. In this work we aim to prove the efficient of some MOF-based catalysts.

2. Materials and Methods

Cerium-, zirconium- and bismuth-based MOFs (MOF-808-Ce, MOF-808-Zr and BiPF-7) were synthesized via one pot solvothermal methods and subsequently shaped into beads using a sodium alginate matrix. Commercial CeO_2 and Bi_2O_3 were used as reference catalysts. The materials were characterized by powder X-ray diffraction (PXRD), N_2-physisorption (BET) and scanning electron microcopy (SEM).

Catalytic tests for the direct synthesis of DMC were performed in a fixed-bed reactor at 100ºC, 9 bar and 13 hours, using CO_2 and methanol. The molar ratio is $CH_3OH/CO_2 = 2$, and the space velocity 61 L/h·g.

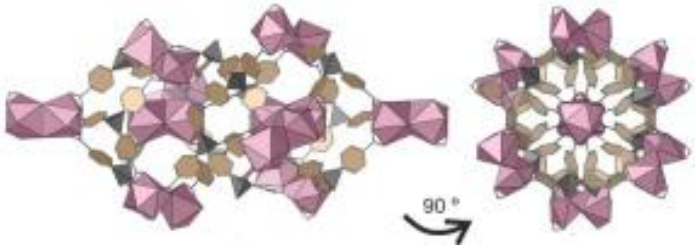


Figure 1. Scheme of the structure of MOF BiPF-7 [3].



3. Results and Discussion

Powder X-ray diffraction patterns confirm the successful synthesis of the targeted MOF structures with high phase purity. Nitrogen physisorption measurements reveal significantly higher specific surface area for MOF-based catalysts compared to their oxide counterparts, while SEM images show smaller particle sizes and more accessible porous morphologies. These features to favor mass transfer and active site accessibility during reaction.

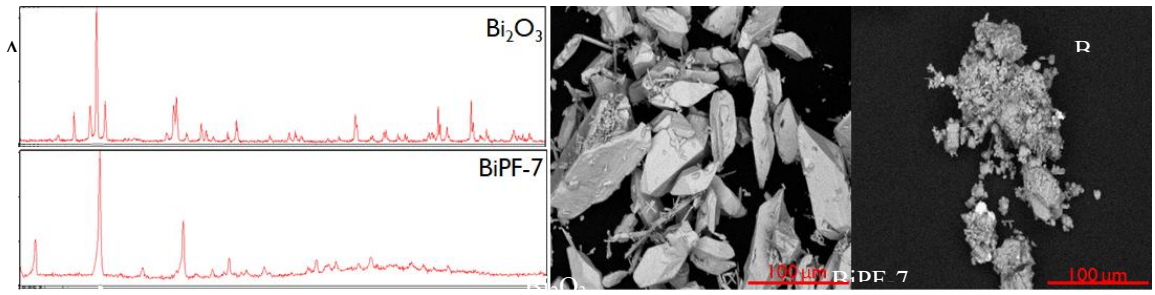


Figure 2. A) PXRD of Bi_2O_3 and BiPF-7; B) SEM micrographs of Bi_2O_3 and BiPF-7.

Catalytic tests demonstrate that MOF-based catalysts outperform the corresponding commercial oxides in the direct synthesis of DMC from CO_2 and methanol. MOF BiPF-7 exhibits the highest DMC production rate, reaching $3.1 \cdot 10^{-02}$ mmol/h·g, attributed to the nature of bismuth active sites, promoting CO_2 activation and methanol polarization.

Table 1. DMC production using different catalysts.

Catalyst	DMC formation rate (mmol / h· g_{cat})
CeO_2	$8.8 \cdot 10^{-03}$
MOF-808-Ce	$1.5 \cdot 10^{-02}$
Bi_2O_3	$1.7 \cdot 10^{-02}$
BiPF-7	**$3.1 \cdot 10^{-02}$**
MOF-808-Zr	$4.6 \cdot 10^{-03}$

4. Conclusions

MOF-based catalysts exhibit superior performance in the direct synthesis of DMC from CO_2 and methanol compared to conventional oxide materials. The enhance activity is associated with higher surface areas and improved accessibility of active sites. Among the studied materials, the bismuth-based MOF BiPF-7 shows the highest DMC productivity, highlighting the potential of MOF structures for efficient CO_2 valorization,

Acknowledgements

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POSSIBILITY OF STEAM ELECTROLYSIS IN DOUBLE SIDED SOLID OXIDE CELLS – (C033)

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Keywords: SOE, steam electrolysis, double sided cells, green hydrogen.

1. Introduction

The development of the hydrogen economy requires the installation of new hydrogen production capacities capable of meeting market demand. Currently, most hydrogen is produced from fossil fuel processing, particularly natural gas through steam methane reforming. Hydrogen production using fossil fuels results in carbon dioxide emissions and other pollutants contained in the fuel (coal gasification, oil reforming). Green hydrogen (emission-free) can be produced in electrolyzers powered by electricity from renewable energy sources or nuclear power plants (purple hydrogen). Among various types of electrolyzers, solid oxide steam electrolyzers (SOC) exhibit the highest energy conversion efficiency from electricity to hydrogen. In typical SOC electrolyzers, cells are constructed as flat plates separated by interconnectors or as tubular cells [1].

The objective of this work was to study the feasibility of using innovative dual-sided SOC cells for the steam electrolysis process.

2. Materials and Methods

In this work, an upscaled dual-sided solid oxide cell manufactured by HydrogenTech, with external dimensions increased to 120 × 70 mm (as compared to the standard cells [2]), was utilized. The cell, compressed between end plates, was placed in a chamber electric furnace. A simplified schematic of the constructed test rig is shown in Figure 1A. A hydrogen-nitrogen mixture (reduction stage) was introduced to the cell's fuel inlet, followed by a mixture of 0.1 Ndm^3/min hydrogen with steam (operation stage). Current-voltage characteristics were recorded, and the hydrogen production rate was measured at temperature ranges of 650–750 °C.

3. Results and Discussion

The current-voltage characteristics obtained for the investigated cell are presented in Figure 1B. During cell operation powered by an electric current of 0–64 A (0–500 mA/cm²), the cell voltage varied in the range of 0.85 to 1.50 V, depending on the measurement temperature and the amount of water vapor supplied to the device.
The lowest voltage required for water decomposition, at the same current density, was observed during operation at a temperature



of 750 °C and a steam flow rate of 50 g/h. The water decomposition voltage in SOEC, ca. 1.20–1.50 V, is lower than the 1.50–1.80 V required for the efficient operation of low-temperature electrolyzers. The reduced operating voltage leads to lower specific energy consumption. At the maximum current densities, the water vapor utilization efficiency reached 86% and 43%, respectively, for steam flow rates of 25 g/h and 50 g/h.

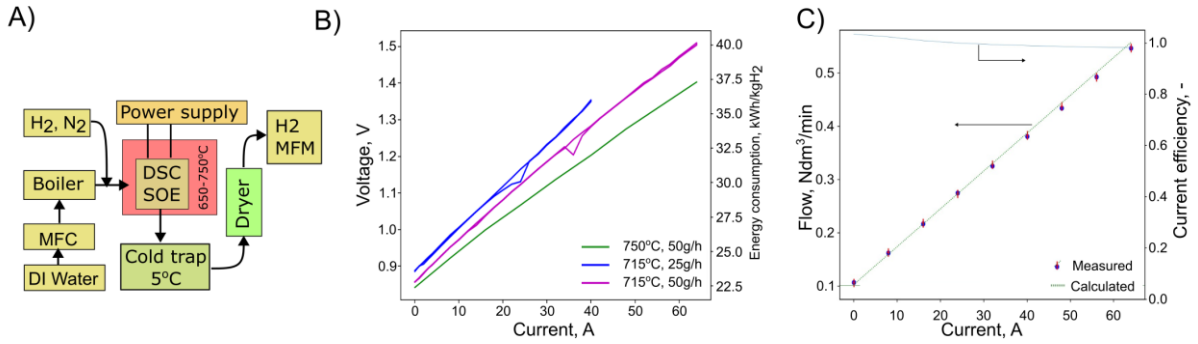


Fig 1. A) experimental setup diagram, B) Current voltage curves recorded for tested cell, C) measured stream of hydrogen produced in tested cell.

The easily sealable design of the DSC enables maintaining gas overpressure in the system and effective hydrogen extraction via a two-stage drying and volume measurement device. The recorded hydrogen flow rate exiting the cell (Fig. 1C) consisted of two components: a) a constant hydrogen feed of 0.1 Ndm³/min serving as a protective gas to shield the anode material from oxidation, and b) the electrolytically generated hydrogen stream, which varied nearly linearly with the current density passing through the electrolyzer.

4. Conclusions

The experiments demonstrate the feasibility of using dual-sided SOE cells for steam electrolysis. The measured hydrogen flux confirms the high faradaic and energy efficiency. The dual-sided design of the investigated cells, combined with the limited length of the fuel channel sealing perimeter, facilitates system sealing, enables elevated operating pressure, and allows efficient recovery of hydrogen produced during electrolysis. The promising results obtained enable the design of SOE cell stacks operating under elevated differential reagent pressures.

Acknowledgements

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FROM PHOTOVOLTAICS TO HYDROGEN TECHNOLOGIES: A UNIVERSAL LSTM-BASED MODEL FOR MARKET DEVELOPMENT FORECASTING – (C034)

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Keywords: distributed energy technologies, hydrogen technologies, time series forecasting, long short-term memory (LSTM).

1. Introduction

The development of hydrogen valleys and energy communities is a key element of the energy transition in the European Union. Although hydrogen technologies are considered an important component of the future energy system, their deployment is limited by high costs and low market maturity. Current research indicates that distributed renewable energy sources play a complementary and transitional role, supporting the stabilization of local energy systems and preparing infrastructure for the integration of hydrogen solutions. This study aims to propose a universal machine learning–based predictive model that can also be adapted for analyses of hydrogen technology development.

2. Materials and Methods

The study is based on the analysis of time series describing the development of the distributed energy technology market. A predictive model using long short-term memory (LSTM) recurrent neural networks was applied to capture temporal and seasonal dependencies. The data included the number of installations and their average capacity at the regional level, and model training and validation were conducted using the mean squared error (MSE) metric. In addition, the model's adaptability to forecasting consumer hydrogen technologies was examined through the redefinition of input and output variables.

3. Results and Discussion

The applied predictive model based on a long short-term memory (LSTM) recurrent neural network demonstrated a high capability to capture the dynamics of the distributed energy technology market. The model accurately reflected both long-term growth trends and short-term seasonal fluctuations in the number of installations and their average capacity, as illustrated by the forecast presented in Figure 1. Compared with classical multilayer perception (MLP) architectures, significantly lower mean squared error (MSE) values were obtained, confirming the superiority of the sequential approach in the analysis of time-dependent market data.

A key feature of the proposed approach is that the model does not represent physical processes related to energy generation, but rather the sequential dynamics of the energy technology market, understood as the outcome of historical investment decisions, deployment structures, and external factors, including seasonality and regional conditions. Consequently, the applicability of the model is not limited to a single technology but extends to a broad class of distributed energy technologies at different stages of market maturity.

The training process was characterized by a rapid decrease in MSE values during the initial training epochs, followed by a gradual stabilization of the error curve, indicating effective model fitting without signs of overfitting (Figure 2). From a methodological perspective, the market for local and consumer hydrogen technologies exhibits significant structural similarities to the photovoltaic market, particularly with respect to the dependence of deployment rates on regulatory and economic factors, the presence of decision-making delays, and pronounced spatial differentiation. This implies the possibility of direct adaptation of the proposed model for forecasting the development of hydrogen technologies, with regionalization retained as an integral component of the analysis.



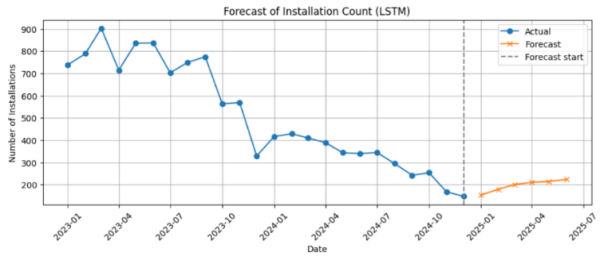


Figure 1. Forecast of the number of photovoltaic (PV) installations based on the LSTM model



Figure 2. Training loss expressed as mean squared error (MSE) over training epochs for the LSTM model

4. Conclusions

The adaptation of the model developed for the photovoltaic market to the analysis of hydrogen technology development does not require major changes to its mathematical structure. It involves redefining input and output variables and calibrating the model using hydrogen-specific data, while preserving the same sequential architecture. As a result, the proposed approach can be considered a universal predictive tool for analyzing the evolutionary development of hybrid energy systems integrating distributed renewable energy sources and hydrogen technologies in a sequential and regionally differentiated manner.

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HIGH-PURITY HYDROGEN PRODUCTION FROM AMMONIA USING INTEGRATED PD–AG MEMBRANE REACTORS WITH STRUCTURED CATALYSTS – (C039)

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Keywords: hydrogen purification, hydrogen carrier; membrane, advanced catalytic structures

1. Introduction

Rising energy demand is accelerating the shift toward clean energy sources. Hydrogen is a promising energy vector, though its transport remains challenging; ammonia represents a viable carrier if efficient decomposition technologies are available. Membrane reactors (MRs) have shown strong potential for ammonia decomposition, typically employing Pd-based membranes due to their high hydrogen selectivity. In this study, a Pd–Ag membrane reactor coupled with a lab-synthesized Ru catalyst supported on $LaCe_2O_7$ was investigated for efficient production and recovery of high-purity hydrogen from ammonia.

2. Materials and Methods

The catalyst, prepared via solution combustion synthesis, was characterised by N_2 physisorption, XRD, H_2-TPR, and TEM. Catalytic layers (0.1g/cm^3) were deposited onto four commercial 30 PPI SiC open-cell foams (o.d.Ø = 9mm, Length = 15mm) using a combined dip–spin coating technique, enabling a comparison between pellet- and structured-based membrane reactors. Reactor performance was assessed under varying pressures and flow rates using pure ammonia or simulated reactor effluents with 20–50% conversion, evaluating hydrogen back-permeation and membrane efficiency. The performance of the MR was evaluated by varying the feed: either only NH_3 or a mixture of NH_3+H_2+N_2. The composition of the mixture corresponds to the outlet of a previous TR, with different conversion.

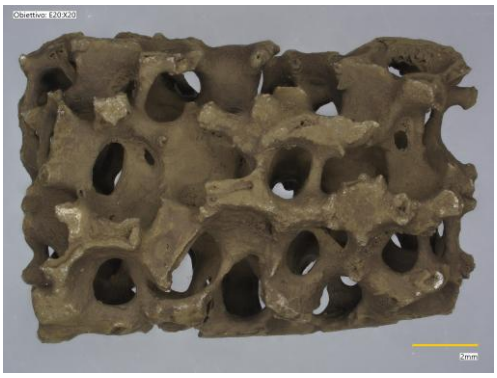
3. Results and Discussion

The proposed strategy to enhance ammonia decomposition in the Pd–Ag MR involves feeding a mixture of NH_3, H_2, and N_2 that simulates the outlet of a partially converted upstream tubular reactor. This approach maintains a positive hydrogen partial pressure along the reactor, mitigating hydrogen back-permeation and improving membrane efficiency. Experiments carried out at 400 °C showed that, for all feed flow rates, NH_3 conversion increased almost linearly with feed pressure, indicating improved MR performance at high pressure despite unfavourable thermodynamics. In all cases, the MR outperformed the traditional reactor, even when feeding mixtures. The highest conversion was achieved at 5 bar with a feed of NH_3+H_2+N_2 = 9.0+3.4+1.1 mL(STP) min^{-1}, approaching or matching the TR thermodynamic equilibrium conversion. The presence of hydrogen enhanced the permeation



driving force, facilitating hydrogen removal and shifting the reaction forward. Higher hydrogen contents also matched or exceeded equilibrium conversion, confirming its beneficial role. However, excess hydrogen (>3.4 mL(STP) min^{-1}) led to reduced conversion due to ammonia dilution and membrane permeation saturation. Hydrogen recovery increased with pressure and hydrogen content, reaching up to 97% at 4 bar, while permeate purity remained above 90%, significantly higher than with ammonia-only feeds. Increasing feed flow rate reduced conversion due to higher GHSV, but recovery and purity decreased only slightly, supported by the increased hydrogen feed.

a)



b)

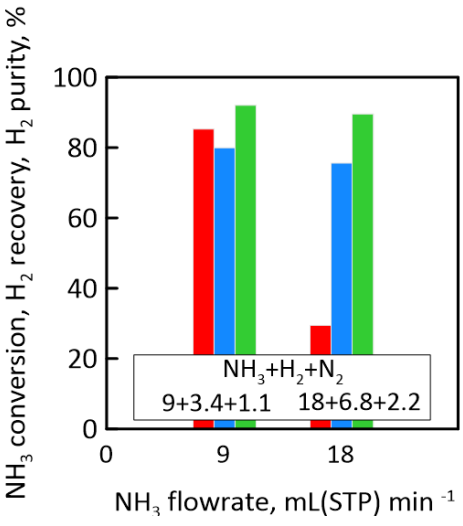


Figure 1. a) Example of a SiC foam activated using the dip/spin coating methodology; b) NH_3 conversion, H_2 recovery and purity at 400°C and 5 bar at different NH_3 feed flow rates.

4. Conclusions

The MR performance improved significantly when feeding a H_2-containing mixture. NH_3 conversion increased with pressure, surpassing TR equilibrium values. H_2 mitigated back-permeation and improved membrane utilization, achieving ~85% conversion at 5 bar and 400 °C, with ~97% H_2 recovery and >90% purity. Compared to the TR, the MR reached up to 3.6-fold higher conversion, confirming its strong potential for efficient ammonia decomposition.

Acknowledgements

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MULTICRITERIA DECISION ANALYSIS METHODOLOGIES: A REVIEW APPLIED TO THE ENERGY SECTOR – (C043)

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Keywords: Multicriteria decision analysis, methodology, Life Cycle Sustainability assessment, energy related technologies

1. Introduction

Performing a Life Cycle Sustainability Assessment (LCSA) in the context of energy related technologies can capture the interactions between different sustainability aspects. Jointly, Multi-Criteria Decision Analysis (MCDA) acts as a methodological bridge by transforming descriptive LCSA results into actionable insights, balancing conflicting criteria with the aim at identifying the best trade-off solution among different alternatives, supporting robust decision-making [1]. This study proposes a review of the current methodological framework used in MCDA to identify trend and critical points in current practices and to provide a structured basis to support future methodological harmonization when MCDA is combined with LCSA in energy applications.

2. Materials and Methods

The present work is based on a structured literature review via Scopus database. First, MCDA theoretical frameworks and clustering criteria for classifying methodologies were identified. Then its applications in the energy sector were systematically identified. Ten case studies were reviewed and analyzed by MCDA phase, weighting and aggregation methods, stakeholder involvement and LCSA integration, allowing identification of recurrent methodological patterns and critical aspects.

3. Results and Discussion

Reviewed works shown that while theoretical reviews identify over thirty distinct MCDA algorithms [2], the landscape changes when focusing on applications in the energy sector, where the spectrum of implemented methodologies narrows significantly. As a result procedural steps may vary by the chosen method, however most studies converge on two partially overlapping macro-phase [3], providing a common reference structure:

- Construction phase: goals & alternatives definition; criteria selection; stakeholder involvement
- Exploitation phase: criteria weighting; criteria aggregation; result comparison.

Focusing on Exploitation given the need for a rigorous methodological framework, established MCDA taxonomies distinguishes compensatory and outranking methods based on the degree of compensability allowed among conflicting criteria. Compensatory approaches like TOPSIS assume full substitutability, whereas outranking methods like PROMETHEE adopt a non-compensatory logic, rejecting alternatives with unacceptable performance in critical criteria, regardless of other merits [2]. The following table lists the ten studies analyzed to evaluate the methodologies applied within Multi-Criteria Decision Analysis (MCDA).



Doi	Field of application	Life cycle techniques	Criteria Weighting	Aggregation Phase	Stakeholder Involvement	Involvment Phase
10.1002/ente.201901019.	Battery Storage Technologies	LCSA, LCC, S-LCA	AHP	TOPSIS	Y	Criteria Selction, Weighting
10.1002/ente.201600622.	Energy Storage	CO_2 Footprint, LCC	Equal weighting	TOPSIS	N	-
10.1016/j.procir.2020.02.124.	Energy	LCA, LCC	Pairwise comparison	TOPSIS	Y	Weighting
10.1007/s10098-022-02407-w	Electric Vehicle	LCSA, LCC, S-LCA	Equal Weighting	TOPSIS	N	-
10.3390/su13137009	Hydrogen Production	LCSA	Equal Weighting	PROMETHEE	N	-
10.1007/978-3-030-77127-0	Hydrogen Production	LCSA	Equal Weighting	PROMETHEE	N	-
10.3390/en18205478	Hydrogen Production	LCSA	IVTFNs	TOPSIS	Y	Criteria Selction, Weighting
10.1016/j.rser.2023.114135	Hydrogen Production	LCA/Techno-economic analysis	-	TOPSIS	N	-
10.1039/D2SE01170K	Hydrogen Mobility	LCSA	SMART	PROMETHEE II	Y	Weighting
10.1007/978-3-031-48359-2_18	Batteries	-	Equal Weighting	PROMETHEE II	N	-

Tab 1 Summary of articles reviewed

Weighting phase reveals equal weighting as the preferred approach; driven by simplicity and no stakeholder consultation needed. Conversely, studies involving stakeholders used diverse participatory methods.

The aggregation phase shows a strong convergence towards two approaches only: TOPSIS and PROMETHEE. These methods differ for the compensatory nature and the algorithm logic. TOPSIS (60% of obs.) minimize the geometrical distance of the preferred alternative from the ideal one, while PROMETHEE (40% of obs.) is based on a pairwise comparison [2]. Finally, all considered



studies also included LCSA; theoretically, LCSA should serve as an input for the subsequent MCDA, where LCA impact categories function as selected criteria and data inputs for performance aggregation. This expected alignment was observed in nearly all case studies, with a subset refining the criteria selection via stakeholder preferences.

4. Conclusions

Although preliminary, the results highlight the need for a clearer methodological framing of MCDA applications in the energy sector. Method selection often favors ease of use over theoretical rigor, in fact in the aggregation phase, TOPSIS prevails due to its accessible compensatory structure. Weighting phase would benefit from broader stakeholder involvement. LCSA integration remains heterogeneous and not always explicitly defined.

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A DUAL SUSTAINABILITY PERSPECTIVE ON PHOTOELECTROLYSIS: INTEGRATED ENVIRONMENTAL AND ECONOMIC LIFE CYCLE ASSESSMENT OF GREEN HYDROGEN PRODUCTION – (C044)

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Keywords: Green Hydrogen, LCA, eLCC, Photoelectrolysis,

1. Introduction

This work consists of a Life Cycle Assessment (LCA), performed according to ISO 14040/44 standards and an environmental LCC (eLCC) [1-2] analysis of a novel photoelectrolysis cell, using a cradle-to-gate approach to help designers make environmentally sustainable and economically viable choices. The calculations were performed on a laboratory prototype cell having an area of 10 cm², and then scaled up to a commercial cell of 80 cm².

2. Materials and Methods

The LCA was conducted using SimaPro 9.6 with Ecoinvent 3 data and the ReCiPe 2016 Midpoint (H) method. The functional unit comprised a single assembled cell, incorporating an anode on FTO glass, a cathode, a polymer membrane and a PVDF casing.

The LCC analysis encompassed the calculation of capital expenditures (CAPEX) and operating expenditures (OPEX). In particular, the Net Present Value (NPV) was calculated in order to assess the economic viability of the investment.

The eLCC was based on the "Environmental Price" (EP) [3] approach, which expresses the willingness to pay for less pollution in euros per kilogram of pollutant considering the Climate change category.

3. Results and Discussion

The results indicate that climate change, human toxicity and terrestrial ecotoxicity are the most relevant impact categories. In normalized terms, human carcinogenic toxicity clearly dominates the environmental profile, reaching a value of $3.34 \cdot 10^{-2}$, followed by freshwater ecotoxicity ($1.31 \cdot 10^{-2}$) and marine ecotoxicity ($9.81 \cdot 10^{-3}$). Terrestrial ecotoxicity also shows a non-negligible contribution ($1.46 \cdot 10^{-3}$), whereas climate change impacts, although relevant ($3.86 \cdot 10^{-4}$), are lower compared to toxicity-related categories (Fig. 1). The primary areas of concern relate to the anode process and fluoropolymer materials, due to high energy consumption and the production of fluorinated compounds. Membrane, casing and assembly stages contribute less significantly.



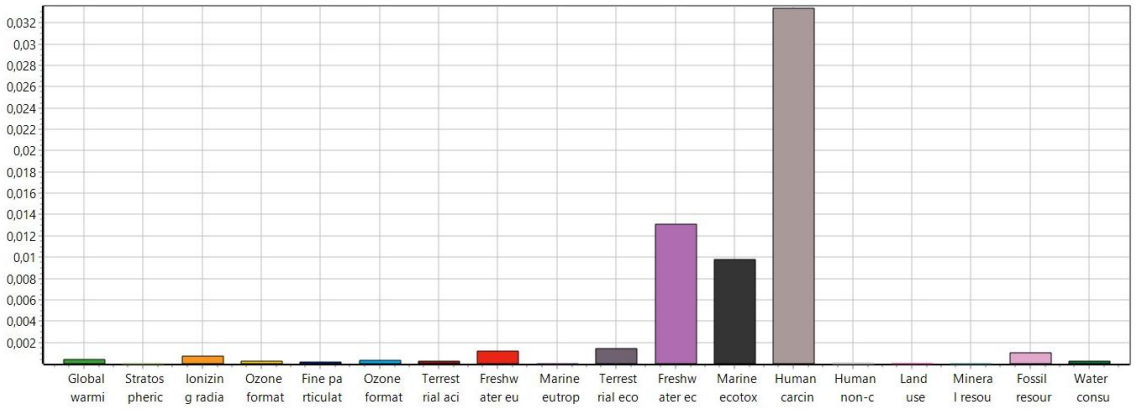


Fig. 1: LCA results using the ReCiPe 2016 midpoint normalised method.

Despite the low technology readiness level (TRL), the study simulated a realistic production and commercialization process. The analysis assumed a semi-artisanal production, with production volumes not exceeding 4,000 units per year. The target market includes not only industry, but also research institutions commissioning cells for experimental applications. In this context, the identification of environmental hotspots provides a consistent basis for the economic assessment, enabling a direct link between environmental burdens and cost drivers within the integrated LCC and NPV analyses. The NPV calculation showed that the break-even point was reached within 3.5 years. Considering externalities as additional costs affecting the production value of the photoelectrolysis cell, the incidence of each cost category is: Capex 91.98%; Opex 7.94%; Climate change (EP) 0.08%.

4. Conclusions

The study emphasises the pressing requirement to minimise the energy intensity of anode production and to replace fluoropolymers with more environmentally friendly alternatives. These measures are essential for steering the development of photoelectrolytic cells towards more sustainable and scalable technologies. To optimise the environmental performance of the device, energy consumption during heat treatments should be limited and the use of low-impact materials integrated.

The product and production process under investigation can be defined as virtuous and sustainable in terms of environmental impact, representing an investment with a good potential return in purely economic terms.

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MACHINE LEARNING-BASED CONTROL OF A SOFC SYSTEM UNDER VARIABLE LOAD CONDITIONS – (C045)

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Keywords: Ammonia fuel, Machine learning control, PID control, Solid Oxide Fuel Cell, SOFC Modeling,

1. Introduction

Solid oxide fuel cells (SOFCs) are highly efficient energy conversion devices, but their performance under variable load conditions strongly depends on the effectiveness of the control system [1,2]. To overcome the limitations of conventional proportional–integral–derivative (PID) controllers, this work proposes a machine learning–based control (MLBC) strategy for hydrogen flow rate regulation in an SOFC system operating under dynamic load conditions. The proposed controller learns the nonlinear relationship between stack current, operating conditions, and fuel demand directly from data, enabling fast and robust control. The application of an intelligent, data-driven control architecture to SOFC load-following operation represents the main novelty of the study.

2. Materials and Methods

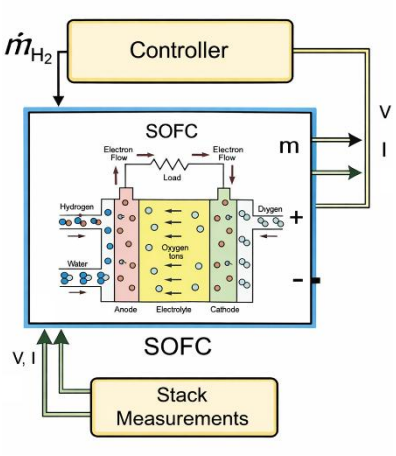
A hierarchical lumped-parameter model was developed in the Simulink environment and validated against experimental data. A feedforward neural network was trained using simulated dynamic data generated from the validated model under a wide range of load conditions. The network inputs include stack current and key operating variables, while the output is the required hydrogen flow rate, to ensure safe and efficient operation.. Moreover, a PID controller was tested under the same conditions.

3. Results and Discussion

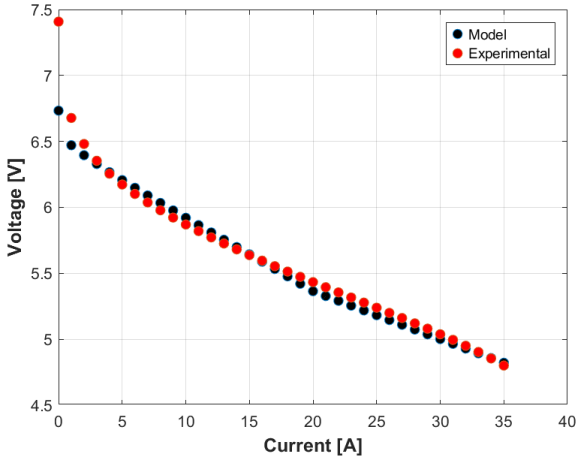
Figure 1a shows the overall SOFC model and control architecture implemented in the Simulink/Matlab environment. The model considers an SOFC stack fueled with a nitrogen–hydrogen (N_2/H_2) mixture obtained from external ammonia reforming. Figure 1b presents a comparison between experimental (red markers) and simulated (blue markers) results for a test carried out at 750 °C. During this test, the SOFC was fuelled with ammonia and air supplied at flow rates of 2.32 lpm and 32 lpm at the anode and cathode, respectively. The simulated results closely match the experimental data over the entire current range, demonstrating the model's ability to accurately reproduce the SOFC electrochemical behavior. Slight deviations observed at high current densities are mainly attributed to increased concentration and ohmic losses, as well as uncertainties associated with fuel utilization and gas composition at elevated loads. Overall, these results confirm that the model is capable of qualitatively and quantitatively describing the dominant physical phenomena governing SOFC operation.

The results confirm clear advantages of the proposed MLBC. In detail, MLBC exhibits faster response times and smoother voltage profiles while the PID controller slower response and larger voltage deviations, especially during rapid current ramps, which may negatively impact stack durability over long-term operation. The comparison highlights how machine learning-based control can outperform classical linear controllers while maintaining low computational complexity, making it suitable for real-time implementation in practical SOFC systems.





(a)



(b)

Figure 1: (a) SOFC/Control system, (b) stack polarization curve at 750 °C.

4. Conclusions

This work presents a neural network–based control strategy for SOFC hydrogen flow regulation under variable load conditions. The validated dynamic model confirms accurate representation of SOFC behavior, while the intelligent controller demonstrates superior transient performance compared to classical PID control. Machine learning–based control represents a promising alternative to traditional and model-based approaches, particularly for SOFC systems operating in highly dynamic energy scenarios.

Acknowledgements

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DESIGN AND VALIDATION OF A 10 CM² TANDEM PHOTOELECTROCHEMICAL PROTOTYPE FOR WATER SPLITTING USING NON-CRITICAL RAW MATERIALS – (C046)

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Keywords: photoelectrochemical water splitting, tandem PEC cell, hematite photoanode, CuO photocathode, anion-exchange membrane.

1. Introduction

Photoelectrochemical (PEC) water splitting is a direct route to solar H_2, but scaling to cm² areas is limited by ohmic drops, current collection and photoelectrode durability. We report a 10 cm² zero-gap tandem PEC cell built only from earth-abundant oxides (α-Fe_2O_3 photoanode/CuO photocathode) and an anion-exchange membrane. The work quantifies module-scale losses via EIS and distribution-of-relaxation-times analysis and assesses 240 h stability and gas purity.

2. Materials and Methods

Nanostructured α-Fe_2O_3 was electrodeposited on FTO and annealed; Cu was electrodeposited on carbon paper, chemically oxidised to $Cu(OH)_2$ and converted to CuO. A PiperION AEM (OH^- form) and matching ionomer layers formed a glass electrode membrane assembly in a PMMA/steel zero-gap prototype (10 cm²).

J–V curves, EIS+DRT, 240 h potentiostatic test (−1.3 V) and Micro-GC were performed under AM 1.5G.

3. Results and Discussion

Under AM 1.5G the tandem delivers a photoresponse already near 0 V and reaches −25 mA cm^{-2} at −1.3 V, giving a maximum hydrogen-production efficiency of 5.1%. EIS shows an area-specific ohmic resistance of ~18 Ω cm², while illumination lowers the interfacial polarization (R_{ct} ~32 Ω cm² at −1.3 V). DRT resolves a dominant millisecond relaxation assigned to charge transfer/double-layer dynamics, with slower contributions emerging at 0 V, consistent with transport/ionic redistribution in the membrane–electrode assembly. A 240-h durability test at −1.3 V maintains nearly constant current; Micro-GC confirms ~99.95% H_2 with O_2 at 0.04–0.06% and no detectable CO/CO_2. Post-operando XRD/SEM show stable hematite, whereas CuO partially reduces and delaminates, identifying the photocathode and series resistance as the main scaling bottlenecks.



Active area	10 cm^2
J at −1.3 V (AM 1.5G)	−25 mA cm^{-2}
H2-production efficiency (max)	5.1% at −1.3 V
Ohmic resistance, R_s (EIS)	~18 Ω cm^2
Charge-transfer resistance, R_{ct} (−1.3 V, light)	~32 Ω cm^2
Durability / H_2 purity	240 h stable; 99.95% H_2 (O_2 0.04–0.06%)

Table 1. Key performance metrics of the 10 cm^2 tandem PEC cell (AM 1.5G, 100 mW cm^{-2}).

4. Conclusions

A bias-assisted 10 cm^2 α-Fe2O3/CuO tandem PEC cell in zero-gap AEM architecture achieves −25 mA cm^{-2} and 5.1% H_2 efficiency at −1.3 V with 99.95% H_2 purity over 240 h. Performance is governed by ~18 Ω cm^2 ohmic loss and CuO instability: future work will focus on reducing ohmic losses and on implementing protected photocathodes.

Acknowledgements

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REALIZATION AND EXPERIMENTAL VALIDATION OF A PEM FUEL CELL STACK OPERATING WITH OXYGEN-ENRICHED FOR NAVAL APPLICATIONS - (C050)

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Keywords: Fuel cell systems for maritime transport, PEM fuel cell stack, Oxygen operation.

1. Introduction

The use of PEM fuel cells in naval applications offers a viable option for reducing emissions and improving energy efficiency in maritime transport. Nevertheless, the marine environment introduces critical challenges related to high humidity and salinity, which can accelerate component degradation and limit the use of ambient air. State-of-the-art solutions therefore rely on controlled oxidant supply and corrosion-resistant materials. Within this framework, this work addresses the design and experimental validation of a PEM fuel cell stack operating under simulated and oxygen-enriched conditions, following a progressive prototyping approach from virtual design to short- and full-stack development.

2. Materials and Methods

The stack was designed to operate with simulated air and oxygen-enriched mixtures. Key components, particularly the membrane electrode assembly, were characterized to optimize membrane thickness and catalyst loading. Electrochemical tests included leakage checks, open-circuit voltage (OCV) measurements, and polarization curve acquisition under controlled flow rates and current loads.

3. Results and Discussion

Preliminary electrochemical characterization of a single cell (Fig. 1) enabled the selection of the most suitable MEA configuration, ensuring an effective balance between performance and durability. The subsequent assembly of a three-cell short-stack was completed without critical issues. Initial leakage tests revealed a gas crossover phenomenon, which was successfully mitigated through a design modification. Polarization curves were then obtained by applying progressively increasing current loads, providing insight into the electrical behaviour of the short-stack under different operating conditions.

Following short-stack validation, a 48-cell PEM fuel cell stack was assembled using graphite–metal bipolar plates, polymer seals, and aluminium end plates to ensure mechanical stability and reduced weight. Uniform compression was applied using steel tie rods and a hydraulic press. The assembled stack was installed on a dedicated test bench equipped with a cell voltage monitoring (CVM) system for real-time diagnostics.

Initial testing confirmed correct operation through OCV measurements with hydrogen and air supply. The stack was then operated under load, with current increased up to 100 A (0.4 A/cm²). Electrochemical characterization was completed by acquiring polarization curves using air and nitrogen–oxygen mixtures with oxygen concentrations of 30% and 100% (Fig. 2).



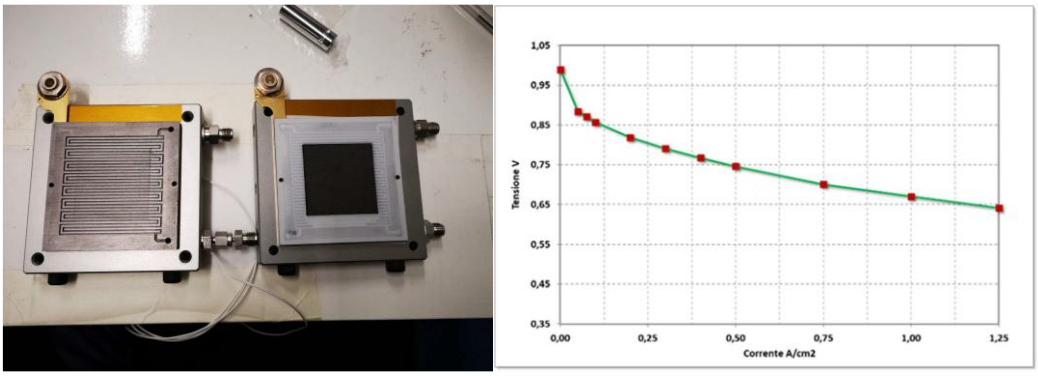


Figure 33 - Single test cell assembly and its experimental polarization curve

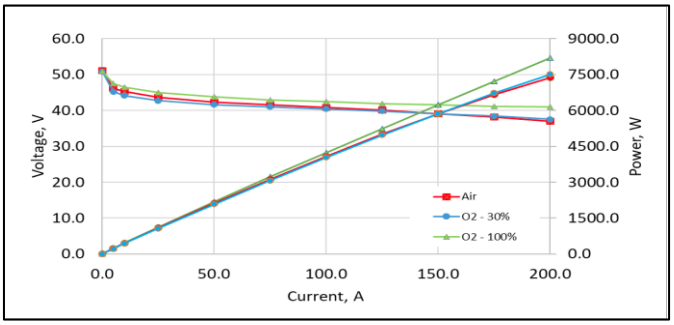


Figure 34 - Polarization curves of the 48-cell stack at different cathode oxygen concentrations.

The results demonstrate stable operation of the stack under all tested conditions. As expected, increasing the oxygen concentration at the cathode leads to improved voltage response and overall performance, confirming the effectiveness of the adopted design strategy for controlled oxidant operation in naval environments.

4. Conclusions

This work presents the design and experimental validation of a PEM fuel cell stack for naval applications operating under controlled oxidant conditions. A stepwise development approach, from virtual modeling to short- and full-stack testing, enabled the definition of suitable materials and operating parameters. The results show stable operation with air and oxygen-enriched mixtures, with improved performance at higher oxygen concentrations, supporting applicability in marine environments.

Acknowledgements

This research was funded by the European Union – NextGeneration EU from the Italian Ministry of Environment and Energy Security POR H2 AdP MMES/ENEA with involvement of CNR and RSE, PNRR - Mission 2, Component 2, Investment 3.5 “Ricerca e sviluppo sull’idrogeno”, CUP: B93C22000630006.

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VIRTUAL ASSEMBLY OF A PEMFC STACK FOR MARINE APPLICATIONS WITH OXYGEN-ENRICHED SIMULATED AIR – (C051)

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Keywords: PEM fuel cell stack, Oxygen-Enriched Cathode, Digital Prototyping

1. Introduction

Polymer Electrolyte Membrane Fuel Cells (PEMFCs) are widely employed in the automotive sector, with configurations optimized for terrestrial mobility. Recently, their potential in naval applications has attracted interest, driven by the need for low-emission propulsion and onboard power. However, marine environments introduce specific constraints, particularly high humidity and salinity, which limit conventional air-fed PEMFC operation and may affect component durability.

To overcome these limitations, alternative oxidant supply strategies are being investigated, including the use of simulated air based on controlled oxygen–nitrogen mixtures. This approach enables operation under conditions compatible with marine environments while supporting efficiency improvements and system integration.

2. Materials and Methods

This activity focuses on the virtual design of a 2-5 kW PEMFC stack for naval use, operating with simulated air and oxygen enrichment up to pure oxygen at the cathode. A digital prototyping approach, combining Computer-Aided Design (CAD) and Computer-Aided Engineering (CAE), was adopted to model and assemble all components. This allowed the verification of interfaces, internal fluid paths, and geometrical constraints related to size, mass, and footprint.

3. Results and Discussion

The virtual assembly resulted in a comprehensive three-dimensional numerical model of the PEMFC stack, allowing early-stage verification of mechanical compatibility and functional coherence among all components. No critical interferences were identified, and the internal hydraulic circuits were confirmed to ensure correct distribution of reactant gases and cooling fluid.

Design optimization carried out at this stage contributed to minimizing volume and weight while maintaining compatibility with oxygen-enriched operation, which imposes stricter requirements in terms of material selection due to increased flammability risks. The use of simulated air also supports system-level benefits, such as reduced onboard gas storage and potential integration with electrolytic hydrogen production, where oxygen is available as a by-product.

Overall, the digital validation phase significantly reduced the risks and uncertainties typically associated with early prototyping, enabling a more efficient transition toward physical manufacturing and experimental testing.

4. Conclusions

A virtual prototype of a PEMFC stack for marine use, compatible with simulated air operation up to 100% oxygen, was successfully developed and validated. The virtual assembly allowed comprehensive pre-manufacturing verification, reducing development time and mitigating early-stage design issues.



These outcomes provide a basis for the subsequent realization of a short-stack and the final 48-cell configuration, supporting the development of high-efficiency (>60%) PEMFC systems for the naval sector.

Acknowledgements

This research was funded by the European Union – NextGeneration EU from the Italian Ministry of Environment and Energy Security POR H2 AdP MMES/ENEA with involvement of CNR and RSE, PNRR - Mission 2, Component 2, Investment 3.5 “Ricerca e sviluppo sull’idrogeno”, CUP: B93C22000630006.

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ENVIRONMENTAL ASSESSMENT OF THE MANUFACTURING PHASE OF AN INNOVATIVE SOFC SYSTEM FED WITH AMMONIA - (C055)

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Keywords: LCA, hydrogen, ammonia, SOFC.

1. Introduction

This study investigates the life cycle environmental profiles of an integrated system composed of a kW scale solid oxide fuel cell (SOFC) stack coupled with an innovative catalytic cracker specifically developed for ammonia decomposition based on structured 3wt.%Ru/CeO_2 catalysts deposited on open-cell ceramic supports. The analysis provides a first LCA-based characterization of the manufacturing phase of the two subsystems, identifying material- and process-related hotspots and supporting eco-design strategies for the development of the first prototype.

2. Materials and Methods

A cradle-to-gate LCA was performed. The functional unit was defined as the complete SOFC–reformer assembly. The inventory was mainly based on primary data provided by the SOFC manufacturer and laboratory activities for the reformer. Environmental impacts were assessed in SimaPro using the Environmental Footprint method, with Ecoinvent as background database and missing substances modelled through stoichiometric reconstruction or appropriate material proxies.

3. Results and Discussion

The assessment revealed that stack assembly (electrodes collectors, end plates, manifolds, insulators, etc..) and system assembly (casing, pipes, heat exchangers, start-up components, etc) represented the dominant environmental burden sources across evaluated categories, with electrochemical cells and the cracker contributing smaller shares (see Table 1).

For climate change (590 kg CO_2 eq total), steel consumption dominated at 75.5% of GHG emissions, reaching 91.8% within stack assembly. Aluminum contributed 9.6%, primarily in heat exchangers. At cell level, bipolar plates accounted for 78.7%, followed by anode (13.3%, driven by nickel at 75% and zirconia oxide at 15%) and cathode (3.3%, from perovskite materials containing cobalt and lanthanum).

Acidification (8.15 mol H^+ eq) was dominated by system assembly (44%), with material hotspots in steel (29.3%), nickel (27.7%), and copper (21.3%). Within cells, the anode contributed most significantly (98% from nickel).Freshwater eutrophication (6.99 kg P eq) showed system assembly as primary contributor (44%). Ferrous materials collectively contributed 58.4%, copper-based materials 19.8%, and brass 14.2%. Metallic interconnectors dominated at cell level.Human toxicity-cancer (1.06E-06 CTUh) concentrated in system assembly (47%). Steel represented the dominant hotspot (57%), followed by copper (17%), brass (13%), aluminum (6.6%), and nickel (5.3%). Bipolar plates and anodes constituted primary cell-level sources.Mineral resource depletion (5.41E-02 kg Sb eq) was dominated by system assembly (70%), primarily from copper (41%), brass (32%), and steel (19%) in piping and connections. Cell-level impacts were driven by nickel in anodes (97% of anode impacts) and steel in bipolar plates.These



findings demonstrate that environmental impacts extend beyond functional electrochemical materials to structural components and assembly architectures, highlighting the necessity of comprehensive eco-design strategies throughout the entire system.

Impact category	Unit	Total	Cell	System assembly	Stack assembly	Reformer
Acidification	mol H+ eq	8.15E+00	1.65E+00	3.58E+00	2.74E+00	1.64E-01
Climate change	kg CO2 eq	5.90E+02	1.16E+02	1.90E+02	2.55E+02	2.97E+01
Ecotoxicity, freshwater	CTUe	9.86E+03	1.66E+03	4.27E+03	3.55E+03	3.75E+02
Eutrophication, fresh.	kg P eq	6.99E-01	1.04E-01	3.10E-01	2.58E-01	2.66E-02
Eutrophication, terr.	mol N eq	8.15E+00	1.37E+00	3.47E+00	2.99E+00	3.23E-01
Human toxicity, cancer	CTUh	1.06E-06	1.58E-07	5.00E-07	3.64E-07	3.51E-08
Resource use, minerals and metals	kg Sb eq	5.41E-02	4.74E-03	3.81E-02	1.05E-02	7.21E-04

Table 1. LCA results of the analyzed system

4. Conclusions

This study identified key environmental hotspots in the SOFC stack/ammonia cracker system. Impacts are dominated by structural assembly choices rather than electrochemical materials, particularly due to steel, copper, and brass use. The cracker showed marginal contribution. Results highlight eco-design opportunities through structural mass reduction and material optimization, providing foundation for future extensions including operational phase and normalized performance assessment.

Acknowledgements

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UNDERGROUND HYDROGEN STORAGE IN DEEP SALINE AQUIFERS: A GEOLOGICAL FEASIBILITY STUDY FOR THE ITALIAN CONTEXT - (C059)

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Keywords: Underground Hydrogen Storage; Deep Saline Aquifers; 3D Geological Modelling; Coupled Fluid-Flow and Geomechanical Simulations; Induced Seismicity.

1. Introduction

The growing penetration of renewable energy requires large-scale, flexible storage solutions to manage seasonal imbalances between production and demand. Green hydrogen is emerging as a key energy carrier for long-duration storage, and geological formations—particularly deep saline aquifers—offer storage potential at the gigawatt- to terawatt-hour scale[1,2]. Given Italy's complex and seismically active geological setting, ensuring containment integrity and controlling pressure-induced stress changes are critical for safe deployment. This work advances current knowledge by integrating high-resolution geological modelling with coupled fluid-dynamic and geomechanical simulations to assess the feasibility of underground hydrogen storage (UHS). The Rivara structure (northern Italy) is used as a representative pilot case to evaluate storage capacity, trapping efficiency, and pressure evolution under cyclic injection-withdrawal scenarios.

2. Materials and Methods

A comprehensive workflow was developed by integrating geological maps, seismic reflection profiles, deep-well data, electrical logs, and technical documentation. These datasets enabled the construction of a 3D geological model used to perform coupled fluid-dynamic and geomechanical simulations supporting the UHS feasibility assessment.

3. Results and Discussion

The Rivara structure exhibits favorable conditions for UHS: hydrogen could be stored within the fractured Noriglio Limestone, vertically sealed by overpressured and low-permeability formations. In addition, this deep saline aquifer is laterally confined by fault zones forming an efficient structural trap (Figure 1). For this reason, a fully integrated 3D geological and structural model was constructed based on seismic interpretation, well analysis, petrophysical assessment (porosity, permeability, and interval velocities properties) and geological cross-sections. The model includes reservoir and seal geometries together with the main tectonic elements (fault surfaces) defining a compartmentalized and structurally framework. Preliminary fluid-dynamic simulations show that pore-pressure increases during injection cycles are mitigated during withdrawal, suggesting stable long-term pressure dynamics and low risk of uncontrolled overpressure. These findings establish a robust basis for the subsequent geomechanical phase, which will quantify stress perturbations and evaluate potential fault reactivation.



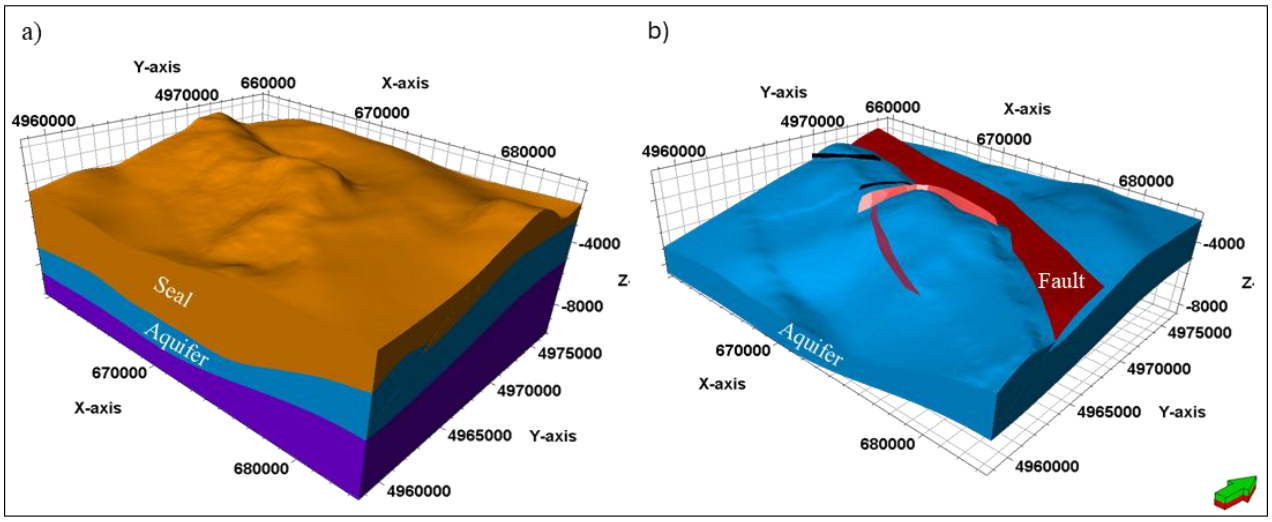


Figure 1. a) 3D view of the aquifer-seal Rivara system; b) Detail of the aquifer with the main structural elements modelled.

4. Conclusions

The integrated geological and numerical approach tested on Rivara structure indicates that deep saline aquifers could be promising for underground hydrogen storage. Preliminary simulations confirm stable pressure behaviour during cyclic operations. These results provide the foundation for upcoming geomechanical modelling, which will assess fault stability and the potential for induced seismicity—an essential step toward evaluating the safety and scalability of UHS in the Italian subsurface.

Acknowledgements

This work has been financed by the Research Fund for the Italian Electrical System under the Three-Year Research Plan 2025-2027 (MASE, Decree n.388 of November 6th, 2024), in compliance with the Decree of April 12th, 2024".

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SEA PLANT DERIVED BIOCARBON AS ELECTROCATALYSTS SUPPORT FOR DMFC - (C065)

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Keywords: Posidonia Oceanica, Activated carbon, DMFC, Biomass-based-Electrocatalyst, LSV.

1. Introduction

Direct methanol fuel cell (DMFC) electrocatalysts are typically composed of Pt or Pt-alloy nanoparticles dispersed onto a suitable support material. The latter plays a crucial role, as it can significantly enhance catalytic activity, improve fuel cell durability and reduce overall system costs. Currently, carbonaceous materials, particularly carbon black, are the most widely used supports. However, many studies have focused on the development of carbon matrices derived from sustainable resources as alternatives to conventional petrochemical-based materials. The present study aims to investigate the performance of DMFC in which both the anode and cathode catalysts are supported on activated carbon derived from a local biomass, Posidonia oceanica, a Mediterranean sea plant.

2. Materials and Methods

Activated carbon was prepared by chemical activation of biomass powder with H_3PO_4 and it was characterized by CHNS analysis, XRD and BET measurements. The obtained activated carbon (AC) was used as a support for Pt and Pt-Ru catalysts, which were characterized by XRD analyses. Electrodes were prepared by spray deposition of catalytic ink on carbon paper and their performance was evaluated in a DMFC.

3. Results and Discussion

The conversion of the starting biomass into activated carbon was confirmed by XRD and CHNS analyses, which evidenced the disappearance of cellulose and calcite crystalline phases along with an increased carbon content. No crystalline phase relative to carbon (i.e., graphite) was detected. BET measurements revealed a micro- and mesoporous structure associated with a high specific surface area, making the material suitable for use as a catalyst support.

Char-supported catalysts were successfully synthesized, as confirmed by XRD analyses, which highlighted the presence of Pt and Pt–Ru crystalline phases in the investigated samples. The detected diffraction peaks ($2\theta = 40°$, 46°, 68°, and 82° for Pt; $2\theta = 43{,}5°$ and 86° for Ru) are consistent with literature data [1]. Electrodes were prepared by spray deposition and tested in a DMFC operating at 90° C with a 2M MeOH solution; and the obtained results are reported in Figure 1.

Figure 1 shows the polarization and power density curves in DMFC, operating in a voltage range between the open circuit voltage (OCV) and 0.05 V. The power density peak is observed at 0.20 V, corresponding to a current density value of 113 mA/cm^2 and a power density value of 23 mW/cm^2.



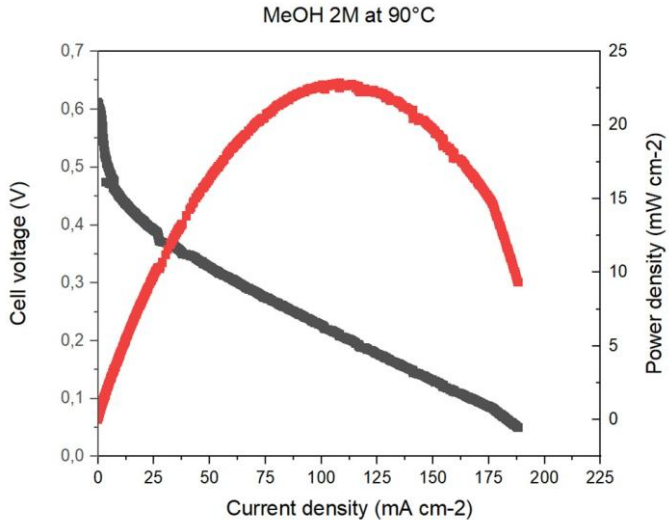


Figure 1: Polarization and power density curves in DMFC for PtRu/AC//Nafion 117//Pt/AC membrane electrode assembly (MEA)

To the best of our knowledge, no literature comparison on DMFC is available in which both electrodes are prepared from biomass-derived activated carbon. Therefore, the above-mentioned results represent a solid foundation for further investigation and open up a wide range of potential future developments.

4. Conclusions

AC from Posidonia was successfully produced by chemical activation, yielding a highly porous structure. The deposition of Pt and Pt–Ru catalysts onto the carbon support was confirmed by XRD results. Electrodes were fabricated by spray deposition; their performance was evaluated by polarization under DMFC operating conditions. This study opens the way to future researches on the use of AC as catalyst supports for various applications, including alcohol electroreforming, PEFCs, water electrolysis.

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SUSTAINABLE MATERIALS FOR HYDROGEN PRODUCTION VIA TANDEM PHOTOELECTROLYSIS AND ALKALINE ELECTROLYSIS - (C067)

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Keywords: Hydrogen, photoelectrolysis, alkaline electrolysis, sustainable materials, earth-abundant catalysts

1. Introduction

The transition toward sustainable energy systems requires the development of efficient and scalable technologies for green hydrogen production. Two of the most promising routes are photoelectrochemical (PEC) water splitting, which directly converts solar energy into chemical energy stored in hydrogen, and alkaline water electrolysis, a mature technology that can be made fully sustainable through the adoption of earth-abundant electrocatalysts. However, the large-scale implementation of both technologies is still limited by several challenges, including low energy conversion efficiency, the use of scarce or critical raw materials and the environmental footprint associated with catalyst manufacturing. For this reason, current research is focusing on tandem PEC architectures based on earth-abundant semiconductors and on alkaline electrolysis cells employing low-cost, sustainable materials such as those derived from volcanic mineral powders and aquatic biomass. In this context, the present work investigates the development of (i) a tandem PEC cell based on hematite (Fe_2O_3) photoanodes and copper oxide (CuO) photocathodes integrated with a polymer electrolyte membrane and (ii) alkaline electrolysis electrodes based on volcanic-derived oxides and aquatic-plant-derived carbon materials.

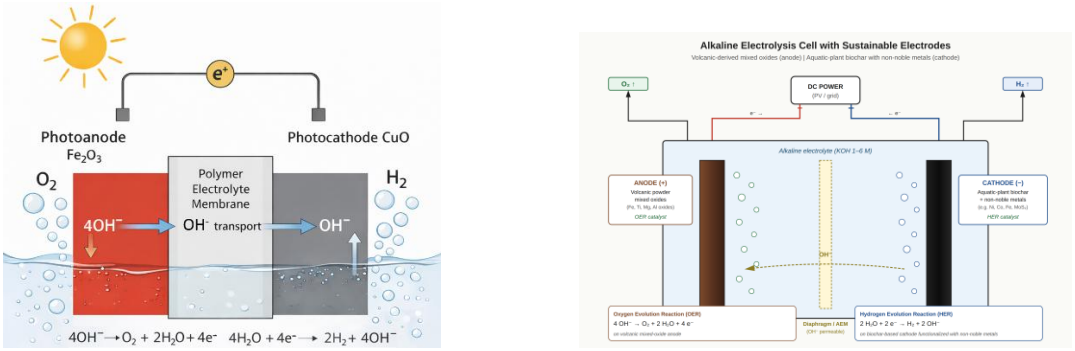


Fig 1. Schematic working principle of tandem PEC and alkaline electrolyzer.

2. Materials and Methods

Nanostructured Fe_2O_3 photoanodes and CuO photocathodes were synthesized using controlled deposition techniques followed by thermal treatments to stabilize the semiconductor phases. In parallel, sustainable electrocatalysts for alkaline electrolysis were prepared starting from naturally available precursors. Volcanic powders, characterized by an intrinsic content of transition-metal oxides (Fe, Ti, Mg, Al), were processed through milling, washing and calcination steps to obtain active catalytic phases for the oxygen evolution reaction (OER). Aquatic plants were collected, dried and pyrolyzed under inert atmosphere to produce biochar-based carbon materials, subsequently functionalized with non-noble metal species to obtain hydrogen evolution reaction (HER)



catalysts. All electrodes were characterized through morphological, structural and surface analyses, and tested through linear sweep voltammetry, electrochemical impedance spectroscopy and chronoamperometry under both photoelectrochemical and alkaline electrolysis conditions.

3. Results and Discussion

The synthesized Fe_2O_3 and CuO electrodes exhibited favorable structural and morphological properties for photoelectrochemical water splitting. The nanostructured architectures provided a large active surface area and enhanced light absorption in the visible region, improving charge carrier generation and interfacial transport. The combination of Fe_2O_3 photoanodes and CuO photocathodes enabled the development of a tandem PEC configuration based entirely on earth-abundant and non-critical raw materials. The device architecture included a polymer electrolyte membrane allowing efficient ionic transport while separating the generated hydrogen and oxygen streams, thus preventing gas crossover and improving operational safety. A prototype PEC device with an active area of 10 cm^2 was fabricated and tested, demonstrating stable hydrogen production with a solar-to-hydrogen efficiency of approximately 5% (Fig. 2) and hydrogen purity higher than 99.9%. In parallel, the materials prepared from volcanic powders and aquatic biomass were evaluated as electrocatalysts in alkaline electrolysis. The volcanic-derived oxides showed promising OER activity, attributable to the synergistic effect of mixed transition-metal oxides naturally present in the precursor and to the porous morphology obtained after thermal activation. The biochar-based catalysts derived from aquatic plants exhibited good electrical conductivity, a hierarchical porous structure and a high density of active sites for HER, especially after functionalization with non-noble transition metals. When integrated in a laboratory-scale alkaline electrolysis cell, these sustainable electrodes delivered current densities and overpotentials competitive with those obtained from conventional reference catalysts, while ensuring stable operation over prolonged tests.

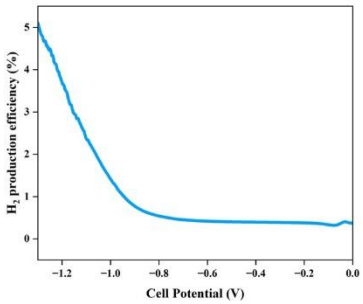


Fig 2. Hydrogen production efficiency of the 10 cm^2 tandem PEC cell as a function of cell potential under simulated sunlight.

Overall, the results highlight how the combined use of earth-abundant semiconductors for PEC devices and of unconventional sustainable precursors (volcanic minerals and aquatic biomass) for alkaline electrolysis can contribute to reducing the dependence on critical raw materials, while supporting circular approaches in hydrogen production technologies.

4. Conclusions

This work demonstrates the development of sustainable hydrogen production technologies based on two complementary approaches: a tandem PEC cell employing Fe_2O_3 photoanodes, CuO photocathodes and a polymer electrolyte membrane, and an alkaline electrolyzer based on electrocatalysts derived from volcanic powders and aquatic plants. The fabricated 10 cm^2 PEC prototype confirmed the feasibility of solar-driven hydrogen generation using non-critical materials, while the alkaline electrolysis tests showed the potential of unconventional, locally available precursors as a viable route toward low-cost and circular electrocatalysts. Future research will focus on the further optimization of device architectures, the scale-up of both systems and the deeper integration of biomass- and mineral-derived materials to enhance performance, durability and environmental sustainability.

Acknowledgements

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ASSESSING ENERGY RESILIENCE OF BUILDINGS AND DISTRICTS UNDER HEATWAVE SCENARIOS: THE CASE OF MONREALE – (C068)

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Keywords: Energy resilience, Heatwaves, Positive Energy Districts, Thermal performance, Urban buildings

1. Introduction

The increasing frequency of heatwaves challenges buildings, urban districts and recent studies highlight the importance of building thermal resilience, understood as the ability to limit the impact of climatic shocks, absorb heat, and restore comfortable indoor conditions during extreme events [1]. At the district scale, Positive Energy Districts promote energy efficiency and renewable integration, but often do not explicitly consider energy resilience under climate uncertainty [2]. Similarly, literature on resilient cooling emphasizes the need to jointly assess buildings and energy systems, considering their capacities to absorb, adapt, and recover [3]. This study aims to evaluate how buildings and energy systems in a district located in the Mediterranean area can be resilient to heatwaves.

2. Materials and Methods

The study proposes the development of a set of key performance indicators and design strategies aimed at quantifying and enhancing building resilience, both in terms of thermal and electrical performance, through the integration of active and passive solutions. The analysis will be conducted on buildings in the Monreale (south Italy, Sicily) district. These tools will enable the identification of the main factors influencing the system's response under extreme conditions.

3. Results and Discussion

Simulations of heatwave scenarios in the Monreale district show that older buildings are more affected by high temperatures and remain in conditions of thermal discomfort for longer periods. Figure 1 illustrates the district under analysis.

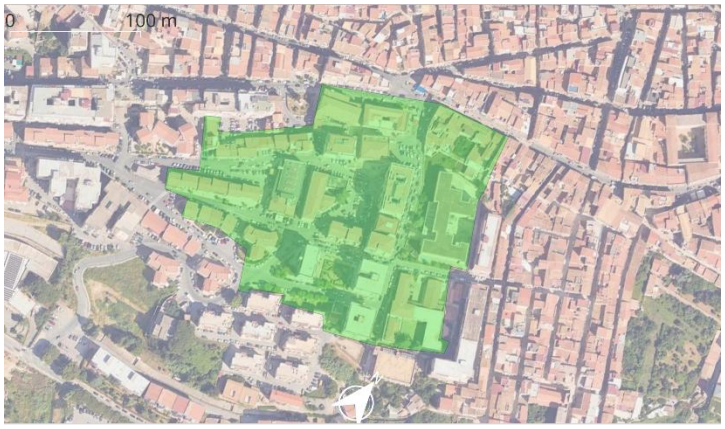


Figure 1. Satellite view of the district



The results highlight significant variability associated both with building geometry and with their spatial distribution within the district. The urban fabric plays a key role in modulating overall performance, influencing energy flows and the local microclimate. At the same time, the intrinsic characteristics of each building, such as materials, insulation, and building systems, determine differentiated responses to thermal and electrical stresses. An integrated approach is needed, considering building design, construction characteristics, operational strategies, and energy management at the district level.

4. Conclusions

The results highlight that the resilience of the Monreale district depends on building characteristics and energy management strategies. An integrated approach at both building and district levels can improve comfort and energy security during heatwaves. The study provides guidance for future interventions aimed at strengthening urban resilience and climate adaptation.

Acknowledgements

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INTEGRATED VOC OXIDATION AND THERMO/PHOTOTHERMO METHANE REFORMING OVER NI/GD-ZR-MODIFIED CERIA - (C070)

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Keywords: VOC, photo-thermo DRM, CO_2 utilization, Ni catalysts, ceria-gadolinia-zirconia.

1. Introduction

Indoor air quality is one of emerging priorities, with VOC emissions from materials, cleaners, and human activities driving the need for effective abatement technologies. At the same time, CO_2 accumulation remains a central global issue, motivating the development of technologies that can not only reduce emissions but also convert CO_2 into value-added products. In this context, thermal and photo-thermal catalytic approaches can be developed for a circular, sustainable and integrated process, where VOCs, in particular toluene, are first oxidized to CO_2 that is subsequently valorized via thermo or photothermo dry reforming of methane (DRM) to produce syngas, thus linking pollutant abatement with carbon utilization within versatile multifunctional catalysts [1]. In this study, Ni catalysts supported on CeO_2 and ceria modified with Gd, Zr, and Gd-Zr are investigated under both thermal and photo-assisted DRM, as well as in the catalytic VOC removal. The aim is to design multifunctional materials that combine enhanced redox functionality with photoresponsiveness, along with improved coking and sintering resistance, applicability to coupled VOC abatement and CO_2 utilization processes [2,3].

2. Materials and Methods

Ni/CeO_2, Ni/CeO_2-Gd_2O_3, Ni/CeO_2-ZrO_2 and Ni/CeO_2-Gd_2O_3-ZrO_2 were synthesized using two distinct methods: a hydrothermal route and a citrate sol-gel route. DRM was carried out in a fixed-bed reactor at 750 °C, after reduction in 5 vol% H_2/Ar at 750 °C for 1 h while photothermo-catalytic reforming tests were carried out at atmospheric pressure in a U-shaped fixed bed quartz reactor, heated by an oven at 500 °C and externally irradiated with a solar lamp, using for both tests 100 mg catalyst and 100 mL min^{-1} CH_4/CO_2/He mixture. For the integrated approach, the most active and stable catalysts were further evaluated for VOC abatement by gas-phase catalytic oxidation at atmospheric pressure. Tests were conducted in a fixed-bed flow reactor, using 0.7 vol% toluene, 10 vol% air and He as balance gas. The reactor was heated with a programmable oven. Reaction products were monitored by gas chromatography coupled with a quadrupole mass spectrometer, enabling quantitative VOC conversion and identification of oxidation products. Samples were characterized by N_2 physisorption, XRD, Raman, XPS, UV-vis DRS, H_2-TPR and CO_2-TPD.

3. Results and Discussion

All catalysts were active for syngas production, with performance strongly governed by support composition and preparation methods. Among the investigated compositions, the $Ce_{0.8}Zr_{0.2}O_{2-x}$ solid solution prepared by hydrothermal method, delivered the highest DRM activity, indicating that Zr incorporation effectively optimizes the redox properties and metal-support synergy of ceria under thermal operation. On the basis of this result, Gd-containing formulations were subsequently investigated to further increase defect density and oxygen exchange capacity, targeting improved carbon management and photothermo responsiveness. Zr incorporation enhanced thermal stability and promoted stronger Ni-support interactions, while Gd introduction increased defect concentration and facilitated oxygen vacancies formation, improving the balance between carbon formation and gasification. The co-modified CeO_2-GdO_x-ZrO_2 support provided the most favorable combination of oxygen mobility and Ni anchoring, translating into improved resistance to coking and sintering during DRM. Under photothermo operation, irradiation further enhanced activity,



consistent with the photoexcitation of ceria-based supports and the promotion of redox cycles that assist reactant activation and surface carbon removal. Considering the integrated approach, toluene was completely converted to CO_2. This is attributed to the higher lattice-oxygen mobility and faster oxygen exchange of the co-doped ceria support compared with the corresponding bare oxides, which enables full conversionf toluene to CO_2.

4. Conclusions

Hydrothermal synthesis enables Ni catalysts on Gd, Zr, and Gd-Zr-modified ceria with tailored redox and photothermal behavior. Co-modification (Gd-Zr) most effectively couples high oxygen mobility with Ni stabilization, strengthening DRM robustness and providing beneficial photo-assistance under simulated sunlight. Overall, the findings show that tuning support composition is the key lever to mitigate coking while sustaining high syngas productivity under both thermal and photothermo operation. In particular, Gd increases defect density and oxygen exchange capacity, whereas Zr improves structural stability and reinforces Ni-support interactions, together facilitating more efficient carbon removal during DRM; under irradiation, accelerated redox cycling further promotes reactant activation and surface carbon cleanup. Finally, these advantages extend beyond DRM, delivering enhanced low-temperature VOC oxidation relative to the bare oxides and achieving complete toluene conversion to CO_2, confirming the broader potential of co-doped ceria formulations.

Acknowledgements

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PYRAZOLE- AND TETRAZOLE-BASED CONDUCTING SALTS FOR SIB ELECTROLYTES - (C077)

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Keywords: SIB, electrolyte, conducting salts, performance, cycling.

1. Introduction

Since the introduction of lithium ion batteries (LIBs), this technology has established itself everywhere in our everyday life and in highly specialized applications. The growing demand for energy storage cannot be met solely by lithium-based technology. Sodium is a promising and abundant alternative for some applications to diversify our resource demand. Given its early stage of development, many aspects remain underexplored. Different state-of-the-art salts for sodium ion battery (SIB) electrolytes like $NaPF_6$, $NaClO_4$, NaTFSI and NaFSI have distinct limitations including low anodic and thermal stability, high cost and low solubility which can limit ionic conductivity at practical concentrations.[1] To face these challenges, we developed and characterized new sodium-based organic salts.

2. Materials and Methods

The Demko-Scharpless synthetic approach by Klapötke *et al.* was used.[2] The solubilities were determined by a gravimetric dissolution method. Furthermore, electrochemical measurements were performed to characterize the performance of each new salt. Those include cyclic voltammetry (CV) and linear sweep voltammetry (LSV) for oxidative/reductive stability assessment, conductivity determination by electrochemical impedance spectroscopy (EIS), and galvanostatic cycling of assembled pouch cells.

3. Results and Discussion

A tetrazole-based sodium conducting salt was prepared according to the above-mentioned method. The tetrazole-based conducting salt (C1) exhibits a wide electrochemical stability window of 0.8 - 4.8 V vs. $Na|Na^+$ (Fig. 1) in the widely used carbonate solvent mixture ethyl carbonate (EC) / diethyl carbonate (DEC) (1:1 wt/wt). Due to the wide electrochemical stability window, this salt is a promising candidate for SIB electrolytes. Additionally, the ionic conductivity was measured and compared to the $NaPF_6$ standard. Due to the solubility of the C1-containing electrolyte being approximately one order of magnitude lower it had a slightly lower conductivity than the $NaPF_6$-based one (Fig. 2).



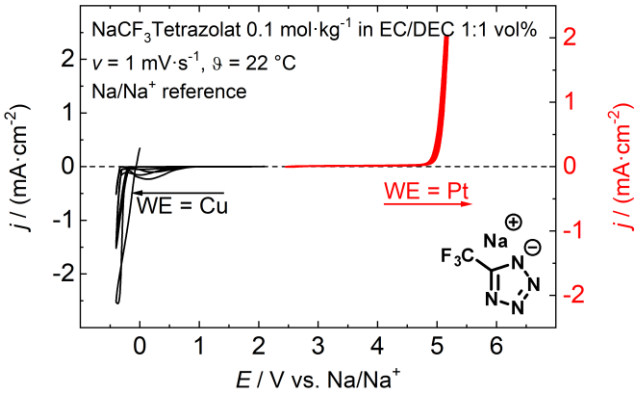


Figure 35: CV measurement of Tetrazole in ethyl carbonate (EC) / diethyl carbonate (DEC).

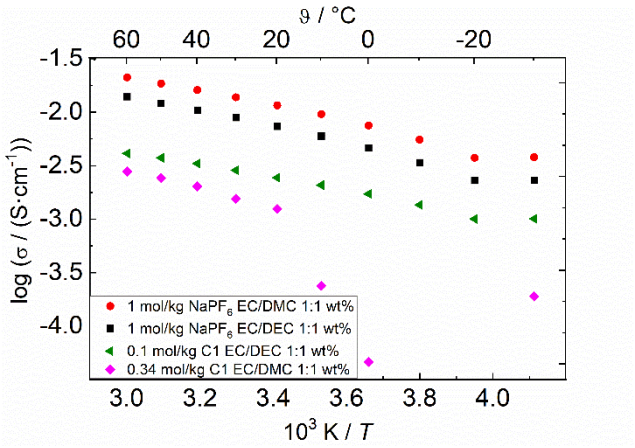


Figure 36: Comparison of conductivities of Tetrazole and the most commonly used $NaPF_6$ as reference measured via EIS.

Since the conductivity is highly dependent on the concentration of the dissolved conducting salt, choosing a different solvent mixture should lead to higher values. Accordingly, we systematically varied the solvent composition for C1 and $NaPF_6$ and benchmarked the resulting electrolytes in half-cells employing two electrochemically distinct cathode materials. Despite only varying the solvent, the two cathodes showed completely different behaviors depending on the electrolyte formulation. Electrolytes based on EC/propylene carbonate (PC) combined with an ether co-solvent performed best overall; however, no stable protective interphase formed (or the interphase was unstable), limiting performance.

4. Conclusions

We synthesized a first promising candidate (C1), evaluated its electrochemical properties, and benchmarked it against $NaPF_6$-based electrolytes. Despite the low solubility this salt class showed very promising results especially if the solubility could be increased in the future by implementing different substituents. Future work will focus on tuning substituents and the core structure to improve solubility while maintaining electrochemical stability.

Acknowledgements

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CRYSTAL PHASE EVOLUTION OF THIN FILMS OF Fe_2O_3 - (C085)

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Keywords: Hematite, Photocatalysis, Water-splitting, Ion-beam sputtering.

1. Introduction

Hematite (α-Fe_2O_3) is a promising material for many applications (e.g. photoanode for solar water-splitting due to its suitable band gap, chemical stability, and abundance). However, its performances are highly dependent on crystallinity and phase purity [1]. Ion beam sputtering offers precise control over thin film growth and a systematic study on phase evolution during post-deposition annealing may offer superior control on phase purity. This work investigates the structural formation of hematite thin films deposited on FTO substrates, focusing on the correlation between annealing conditions, crystallinity, composition, morphology, and electrochemical performance.

2. Materials and Methods

Fe_2O_3 thin films were deposited on 1cm^2 FTO substrates by ion beam sputtering. Isochronal and isothermal annealing treatments were applied to promote hematite phase formation. Structural evolution was analyzed by X-ray diffraction (XRD) at low angle. Composition was determined using Rutherford backscattering spectroscopy (RBS), morphology by SEM, and electrochemical characteristics trough Electrochemical Impedance Spectroscopy (EIS).

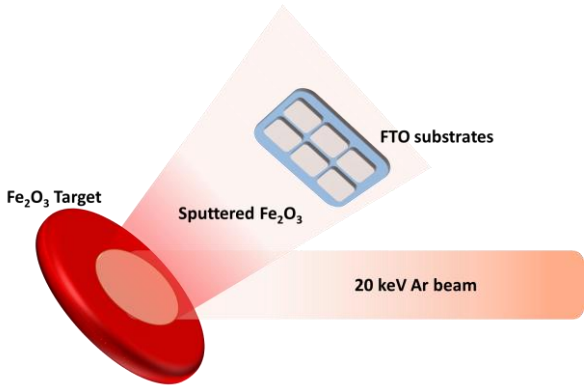


Figure 37 - Schematic representation of the synthesis process



3. Results and Discussion

The samples obtained thermally treated at different temperatures showed differences in surface morphology of the thin iron oxide layer and degree of crystallinity

4. Conclusions

Ion beam sputtering of a thin film of Iron Oxide allowed for the synthesis of photoelectrodes with a uniform active layer with fine control on the thickness. Thermal treatments of the samples after the deposition allowed for the alteration of the morphology, crystallinity and electrochemical properties of the films for the improvement of the electrode performance. These results could lead to better performing photoanodes that are also easily scalable in surface area thanks to the IBS technique.

Acknowledgements

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ENGINEERING BIOCHAR AS A DUAL-FUNCTION CARBON PLATFORM FOR SODIUM/LITHIUM STORAGE AND ELECTROCHEMICAL SENSING - (C101)

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Keywords: Biochar, lithium-ion batteries, sodium-ion batteries, electrochemical sensing, sustainable carbon materials.

1. Introduction

Electroanalytical devices increasingly rely on carbon nanomaterials such as graphene and CNTs, whose production is energy-intensive and environmentally burdensome [1-2]. Biochar, obtained from biomass pyrolysis, represents a low-cost and sustainable alternative with tunable surface chemistry and porosity. However, the relationship between pyrolysis-induced structure and electroanalytical performance remains insufficiently clarified [3-4]. This work demonstrates that pyrolysis temperature alone enables structure-driven optimisation of biochar as a single sustainable carbon platform for both battery anodes (LIBs/NIBs) and high-performance electrochemical sensing.

2. Materials and Methods

Biochars were produced from different lignocellulosic biomass by controlled pyrolysis (700-800 °C). Materials were characterised by SEM, Raman spectroscopy and BET analysis. Anodes and Screen-printed electrodes were fabricated using biochar-based inks and evaluated using Galvanostatic Charge-Discharge (GCD) Cycling, cyclic voltammetry, electrochemical impedance spectroscopy, and differential pulse voltammetry with standard redox probes and model analytes.

3. Results and Discussion

Increasing pyrolysis temperature progressively enhanced structural ordering, reduced oxygen functionalities and improved electrical conductivity. Low-temperature biochars showed high surface reactivity but limited electronic transport, whereas intermediate-temperature materials (600–800 °C) provided the best balance between conductivity, defect density and hierarchical porosity.

As anode materials, these biochars exhibited improved charge-transfer kinetics and stable cycling in both lithium-ion and sodium-ion systems. The turbostratic structure enabled efficient ion diffusion, while defects and residual heteroatoms contributed additional storage sites.

In electroanalysis, biochar-modified electrodes showed faster heterogeneous electron transfer, lower charge-transfer resistance and improved analytical sensitivity compared with conventional carbon inks.



The enhanced performance across applications originates from common structural features—interconnected porosity for mass transport, defect-mediated charge transfer and functional surfaces for interfacial interactions—demonstrating that pyrolysis engineering enables multifunctional optimisation without complex nanomaterial synthesis.

4. Conclusions

Pyrolysis-engineered biochar enables structure-controlled optimisation of electrochemical behaviour across different technologies. Intermediate-temperature materials provide the optimal compromise between conductivity, defects and porosity, supporting efficient ion storage in LIBs/NIBs and rapid electron transfer in sensing platforms. The results identify biochar as a scalable, low-cost and circular carbon material capable of replacing conventional nanocarbons in multifunctional electrochemical devices.

Acknowledgements

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LOW-COST TI-DOPED HEMATITE AND $Cu_2Cr_2O_5$ PHOTOELECTRODES FOR TANDEM PHOTOELECTROCHEMICAL HYDROGEN PRODUCTION - (C106)

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Keywords: photoelectrochemical water splitting, solar hydrogen, hematite, copper chromite, tandem PEC.

1. Introduction

Photoelectrochemical (PEC) water splitting is a promising route to produce green hydrogen, but the cost and stability of photoelectrodes limit large-scale deployment [1, 2]. State-of-the-art systems often rely on scarce or unstable materials. Earth-abundant metal oxides such as hematite and copper-based oxides are attractive, yet they suffer from recombination losses and durability issues. This work aims to develop low-cost and stable oxide-based photoelectrodes and to evaluate their integration in tandem PEC cells for efficient solar hydrogen production.

2. Materials and Methods

$Cu_2Cr_2O_5$ powders were synthesized by precipitation from ammonium dichromate and copper nitrate, followed by drying and calcination at 500 °C. Photocathodes were prepared by spray-depositing CuO or $Cu_2Cr_2O_5$ inks onto gas diffusion layers. Ti-doped α-Fe_2O_3 photoanodes were fabricated on FTO via hydrothermal growth of FeOOH, Ti doping, and annealing at 650 °C. XRD, SEM, and UV–Vis were used for characterization, and PEC tests were performed in half cells and tandem cells.

3. Results and Discussion

XRD and UV–Vis analyses confirmed the formation of Ti-doped hematite with a band gap of 2.1–2.3 eV and broad visible absorption. SEM showed a nanocolumnar morphology that favors charge transport and reduces recombination. In half-cell tests under 1 M KOH, Ti-doped hematite delivered photocurrents about four times higher than Zr-doped hematite. The addition of NiFeOx and Pt co-catalysts did not yield significant improvements.

Both CuO/GDL and $Cu_2Cr_2O_5$/GDL photocathodes were photoactive, but $Cu_2Cr_2O_5$ exhibited higher photocurrents at comparable potentials. Tandem PEC cells were assembled using Ti-doped hematite as photoanode and CuO or $Cu_2Cr_2O_5$ as photocathode, separated by an anion-exchange membrane (FAA3-50, Fumatech). The Ti-hematite/$Cu_2Cr_2O_5$ configuration showed the best performance, reaching ~10 mA cm^{-2} under illumination and a photocurrent of −8.74 mA cm^{-2} at 1.3 V. These results indicate that copper chromite is a more effective and stable photocathode than CuO when paired with Ti-doped hematite.



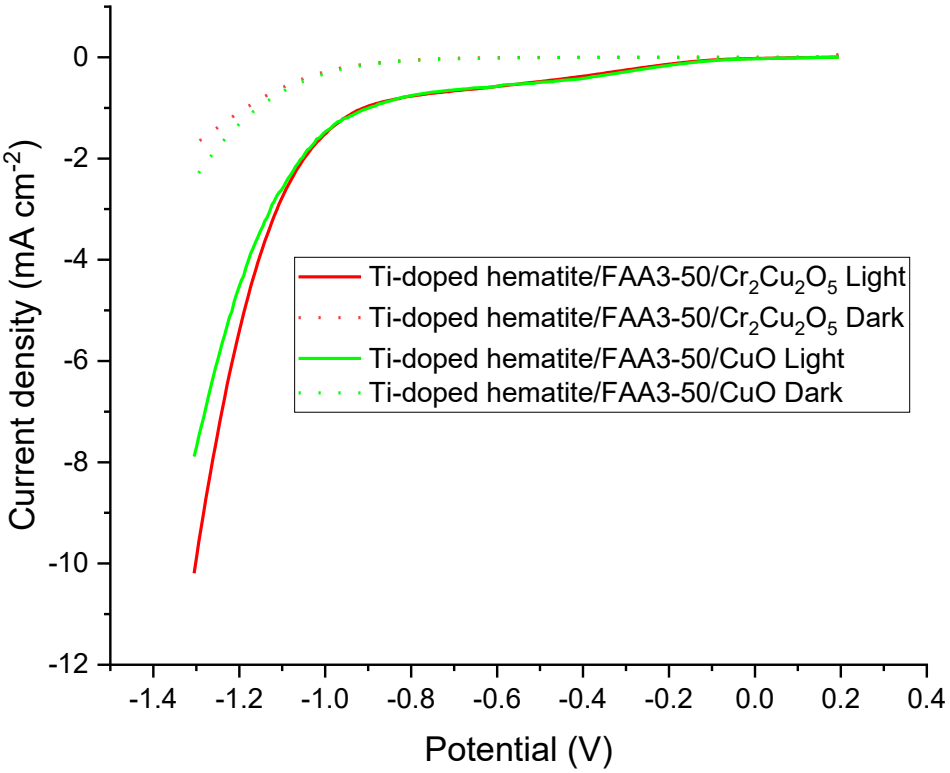


Figure 1. Polarization under illumination and in the dark of the two tandem PEC based on CuO or $Cr_2Cu_2O_5$ photocathode

4. Conclusions

Ti-doped hematite and $Cu_2Cr_2O_5$ form a promising, low-cost photoelectrode pair for PEC hydrogen production. Ti doping strongly enhances hematite performance, while $Cu_2Cr_2O_5$ outperforms CuO as a photocathode. Future work will target long-term stability and interface engineering to further increase solar-to-hydrogen efficiency.

Acknowledgements

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DIGITAL TWIN FRAMEWORK FOR PRE-DEPLOYMENT PLANNING OF THE H2TALENT GREEN HYDROGEN VALLEY IN ALENTEJO - (C108)

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Keywords: Hydrogen Value Chain, Techno-Economic Analysis, Multi-Sector Integration, Energy Communities

1. Introduction

European hydrogen valleys are advancing from concept to deployment where digital twin methodologies have emerged as pre-deployment tools, with e.g. HyModelica in Aragon developing frameworks for renewable hydrogen plant modeling [1], and electrolyzer fleet digital twins demonstrating optimization capabilities [2]. However, most reported digital twins address single-component optimization rather than multi-site valley ecosystems. This work presents an overview of the different demonstrators and their characteristics as well as a digital twin framework under development of the H2tALENT Green Hydrogen Valley in Portugal's Alentejo region. Primary focus will be on Culatra Island's renewable energy community where system design is accomplished and implementation is ongoing.

2. Materials and Methods

A framework integrating Hexagon software, a MYSQL database and Python scripts implementing scheduled workflows, processes real-time web API inputs through an economic engine, accessible through a graphical dashboard. Techo-economic metrics encompass CAPEX/OPEX, LCOE, LCOH calculations. Four sites encompass the value chain: Sines (15 MW electrolyzer, up to 100 bar grid injection), Alandroal (350 bar refueling station, 2 buses), Évora (H_2-NG blending up to 20% H_2) and Culatra Island (5.5 kW electrolyzer, 5 kg storage, 10 kW fuel cell).

3. Results and Discussion

The dashboard enables pre-deployment modeling across production scales (5.5 kW-15 MW), storage pressures (30-500 bar), and various end-use sectors. Performance indicators tracked via MySQL include system efficiency, individual component performance (electrolyzer, compression, fuel cell), state-of-charge, load factor, renewable energy self-sufficiency. Economic indicators encomass levelized costs, NPV sensitivity, payback periods, and unit production costs. The hydrogen containerized system at Culatra Island has been designed, with installation scheduled for Q4 2026. For this demonstrator, scenario definition interfacing with the Energy Management System can balance production during solar availability with dispatch for baseload power. For Alandroal mobility, the framework models refueling utilization with tube trailer logistics, compression energy (estimates 22 kW for 7.5 kg/h), and fleet demand (2 buses, 50000 km/year). Sines' modeling assesses grid electricity costs under renewable certification, compression to 100



bar for National Gas Network injection via hydrogen Backbone, and hydrogen sales revenue that includes injection and tube trail filling for hydrogen road transportation. Évora's blending evaluates mixture flow rates (12.9-14.0 Nm3/h for 10-20% hydrogen), hydrogen injection and energy content adjustments maintaining burner performance for swimming pool heating. Cross-site integration reveals synergies where Sines MW-scale production could supply Alandroal via tube trailer or Évora via bundle supply logistics.

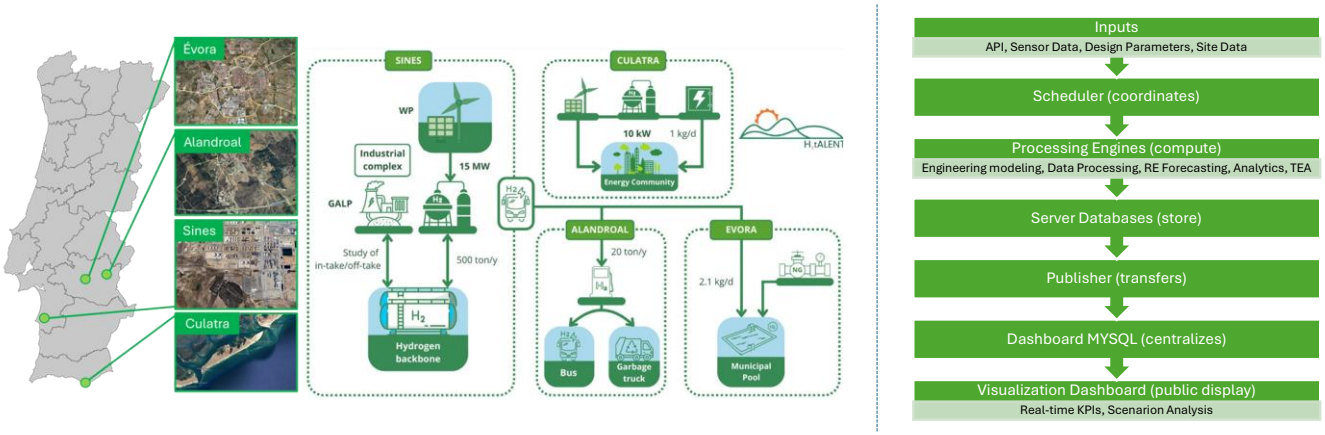


Figure 1. (left) Geographical locations and hydrogen chain in H2tALENT project and (right) preliminary dashboard integration workflow.

4. Conclusions

The Hexagon-Python digital twin framework with integrated MySQL database and accessible through an operational dashboard demonstrates pre-deployment planning capabilities for multi-site hydrogen ecosystems. The scheduled workflow architecture enables real-time techno-economic assessment through API-driven data intake and automated scenario processing. The methodology enables design evaluation, economic analysis, and integration opportunities before construction. Scenario modeling reveals potential for component optimization and regional synergies. Future work includes validation against operational data after the deployment of the first demonstrator (Culatra Island), following the other demonstrators and real-time SCADA integration into the operational dashboard system.

Acknowledgements

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STRUCTURE-ACTIVITY RELATIONSHIPS IN Mg-DOPED $LaNiO_3$-DERIVED CATALYSTS FOR LOW-TEMPERATURE AMMONIA DECOMPOSITION - (C109)

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Keywords: Ammonia decomposition, perovskite, nickel, kinetics, hydrogen

1. Introduction

Ammonia is a promising carbon-free hydrogen carrier and a key enabler of a sustainable hydrogen economy, making the design of efficient catalysts from earth-abundant materials essential to lower costs [1]. Nickel-based perovskites have emerged as attractive alternatives to conventional Ru catalysts, owing to their low cost and their ability to generate highly dispersed metallic Ni nanoparticles via exsolution during reduction [2]. This work investigates Mg-doped $LaNiO_3$ perovskites as catalyst precursors for ammonia decomposition, elucidating how Mg incorporation tunes their structural, redox and catalytic properties and governs the reaction kinetics and mechanism, providing structure–activity insights for low-temperature hydrogen production.

2. Materials and Methods

$La_{1-x}Mg_xNiO_3$ perovskites (x = 0, 0.3, 0.6 and 0.9) were synthesized by sol-gel combustion [3] and characterized by structural and redox techniques. Kinetic tests were performed at 400–450 °C by varying NH_3, H_2 and N_2 concentrations at a GHSV of 60,000 cm^3 g^{-1} h^{-1}. Data were fitted with power-law and Bradford models. The mechanism was probed by in-situ NH_3-TPD coupled with DRIFTS.

3. Results and Discussion

Mg incorporation progressively modified the rhombohedral $LaNiO_3$ framework, favouring Mg-Ni oxide phases and stabilizing small metallic Ni particles after reduction. For the most Mg-rich catalyst, $La_{0.1}Mg_{0.9}NiO_3$, Ni crystallites of ca. 7 nm were obtained, providing a high density of accessible active sites. This catalyst showed the highest activity, and kinetic analysis indicated that the recombinative desorption of adsorbed nitrogen species (N*) is the rate-determining step. In-situ DRIFTS of NH_3 decomposition over $La_{0.1}Mg_{0.9}NiO_3$ (Figure 1) evidenced bands assigned to NH_3 coordinated on Lewis acid sites and NH_4^+ species on Bronsted acid sites. Upon heating, the progressive decrease of adsorbed NH_3 bands and the growth of features related to -NH_2 and -NH intermediates confirmed stepwise ammonia dehydrogenation. Since these NH_x species were already formed at relatively low temperature, the dehydrogenation steps are unlikely to control the overall rate. Conversely, the persistence of surface nitrogen species and the delayed evolution of N_2 support nitrogen recombination/desorption as the most critical step. Mg addition enhances the electron-donating character and basicity of the catalyst surface, facilitating NH_3 activation as well as N_2/H_2 removal, thereby improving low-temperature ammonia cracking performance.



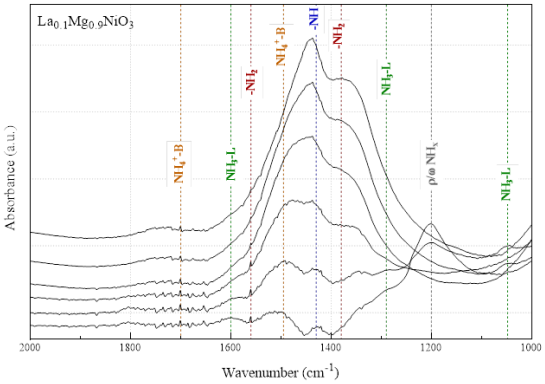


Figure 1. In-situ DRIFTS spectra collected during NH_3 decomposition over reduced $La_{0.1}Mg_{0.9}NiO_3$.

4. Conclusions

Mg-doped $LaNiO_3$-derived catalysts are effective Ni-based systems for low-temperature ammonia cracking. The best performance was obtained for $La_{0.1}Mg_{0.9}NiO_3$, where Mg promoted Ni dispersion, surface basicity and favourable kinetic behaviour. Spectroscopic and kinetic evidence consistently identify nitrogen recombination/desorption as the key limiting step, highlighting Mg doping as a useful strategy to tune Ni-based perovskite-derived catalysts for hydrogen production from ammonia.

Acknowledgements

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SYNTHESIS AND CHARACTERIZATION OF NASICON-BASED ELECTROLYTES DOPED WITH TRANSITION METALS - (C110)

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Keywords: NASICON, battery, metal, doping.

1. Introduction

Sodium batteries are emerging as a promising technology for large-scale energy storage due to the high abundance and relatively low cost of sodium compared to lithium. Among them, solid-state Na-ion batteries are gaining attention for their improved safety and higher energy density. A key component in these batteries is the electrolyte, and NaSiCON (Natrium Super Ionic CONductors) solid electrolytes are considered leading materials in this field. NaSiCON exhibits a crystalline structure that allows high sodium-ion mobility, with ionic conductivity exceeding 10^-4 S/cm at room temperature. This conductivity can be further enhanced by doping with transition metals such as Fe, Co, and Ni, which create active sites and structural defects that facilitate ion transport [1]. However, synthesizing doped NaSiCON presents challenges: reaction parameters must be precisely controlled to avoid secondary phases, dopant distribution must be uniform to ensure consistent electrochemical properties, and chemical and thermal stability must be maintained to guarantee long-term performance.

2. Materials and Methods

NASICON electrolytes doped with Co, Ni, and Fe are synthesized by solid-state reaction using ball milling. The powders are calcined at 1000–1150 °C and sintered at 1150 °C in a muffle furnace. Phase formation is analyzed by XRD, thermal stability by TGA/DSC, and ionic conductivity by electrochemical impedance spectroscopy.

3. Results and Discussion

XRD analysis revealed a strong dependence of phase purity on both dopant type and calcination temperature. Co-doped samples showed a maximum NASICON phase fraction of 67.7% at 1150 °C, with significant secondary phases (ZrO_2, $ZrSiO_4$, Na_3PO_4), indicating incomplete phase stabilization. Fe-doped materials exhibited higher NASICON content at lower temperature (90.6% at 1000 °C), but impurity levels increased upon heating, suggesting thermal instability of the Fe-containing system. In contrast, Ni-doped samples demonstrated the highest structural stability, reaching 94.4% NASICON phase at 1150 °C with minimal secondary phases (5.6%). These results indicate that Ni substitution more effectively stabilizes the NASICON framework compared to Co and Fe.

TGA/DSC measurements of samples calcined at 1150 °C showed negligible mass loss and only high-temperature endothermic events, confirming good thermal stability of the crystalline framework. During sintering at 1150 °C,

Co- and Fe-doped pellets exhibited partial melting and macroscopic degradation, preventing reliable electrochemical characterization. Conversely, the Ni-doped sample maintained structural integrity and was further analyzed by electrochemical impedance spectroscopy in the −20 to 140 °C range. Nyquist plots showed the typical high-frequency semicircle associated with bulk ionic conduction, progressively decreasing with increasing temperature. The total ionic conductivity followed Arrhenius behavior (Table 1), reaching 8.43×10^{-4} S·cm^{-1} at room temperature and 1.35×10^{-2} S·cm^{-1} at 120 °C. These values are comparable



to high-performing undoped NASICON systems, demonstrating that Ni doping preserves high ionic transport while ensuring good phase purity.

Temperatura (°C)	*Conducibilità σ (S·cm^{-1})*
	NaS-Ni
-20	*1,04E-04*
0	*2,76E-04*
20	*6,91E-04*
RT (25)	*8,43E-04*
40	*1,39E-03*
60	*2,70E-03*
80	*4,90E-03*
100	*8,09E-03*
120	*1,35E-02*
140	*2,02E-02*

Table 1. Ion conductivity values of the NaS-Ni sample at different temperatures obtained from electrochemical impedance spectroscopy measurements.

4. Conclusions

Ni doping proved to be the most effective strategy to stabilize the NASICON structure, achieving 94.4% phase purity and high ionic conductivity (8.43×10^{-4} S·cm^{-1} at RT). Co and Fe substitutions led to secondary phases and sintering instability. Ni-doped NASICON represents a promising candidate for solid-state sodium-ion conductors.

Acknowledgements

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MARKET-DRIVEN ROLLING DAY-AHEAD OPTIMIZATION OF HYDROPOWER REVENUES THROUGH FLEXIBLE ELECTRICITY AND HYDROGEN PRODUCTION – (C111)

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Keywords: Optimization, Hydropower, Green Hydrogen, Flexibility

The increasing penetration of renewable energy sources, together with the decarbonization targets set by the Fit for 55 and REPowerEU programmes, is reshaping the European electricity market. Power prices are becoming increasingly volatile, and the system is progressively relying on highly flexible generation technologies, such as gas turbines, to ensure grid stability. In this context, diversifying the product portfolio and enabling flexible plant operation may represent a strategic opportunity. In particular, coupling renewable electricity generation with green hydrogen production could enhance profitability while contributing to the emerging hydrogen market. Hydropower offers a unique advantage in this scenario: it provides zero-carbon electricity with relatively stable output levels. Building on these characteristics, this work investigates market-oriented decision-making strategies for the joint production of hydrogen and electricity from an existing 20 MW_el hydropower plant located in the Trentino region (Northern Italy). The main objective is to assess whether integrating a water electrolysis unit can increase the overall profitability of the plant. To this end, a rolling day-ahead optimization framework has been developed to maximize the operator's annual profit. Monthly fixed-price hydrogen delivery contracts are assumed, while electricity is traded on the day-ahead market. The performance of the integrated and flexibly operated configuration is compared with two reference cases: the stand-alone hydropower plant and a retrofitted configuration operating under a fixed production strategy (hydrogen to power). Finally, sensitivity analyses are carried out to evaluate the impact of hydrogen contract intensity, hydrogen selling price, and switching frequency between electricity and hydrogen production.

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EFFECT OF REACTION PARAMETERS ON CRACKING AND SELECTIVE CATALYTIC DEOXYGENATION OF BIO-OIL MODEL COMPOUND TO PRODUCE RENEWABLE FUEL OVER NI-BASED SUSTAINABLE CATALYSTS - (C112)

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Keywords: Biomass-derived bio-oil, upgrading, Hydrodeoxygenation, Heterogeneous catalysis, Ni catalysts.

Introduction

Bio-oil obtained from fast pyrolysis of biomass, particularly lignin-rich fractions, represents a promising intermediate to produce diesel range hydrocarbons (>C_{11} - C_{20}). It differs significantly from conventional diesel due to its high oxygen content (10 - 40 wt.%), elevated moisture content (15 - 30 wt.%), and much lower heating value (≈17 - 24 MJ kg^{-1}, compared to ≈42 - 46 MJ kg^{-1} for commercial diesel), which necessitates upgrading processes prior to utilization [1].

Among the valorization strategies, two main pathways are commonly reported for bio-oil deoxygenation: (a) catalytic cracking, and (b) catalytic hydrodeoxygenation [2,3]. Catalytic cracking is typically carried out at high temperatures (400 - 500°C) using acidic zeolitic catalysts; however, excessive coke formation (>20 wt.%) may occur on the catalyst surface leading to shorter catalyst lifetime and low selectivity and yield. On the other hand, hydrodeoxygenation operates under H_2-rich atmospheres, moderate pressure (10 - 30 bar), and temperatures (250 – 400°C), using selective and stable heterogenous catalysts to remove oxygen from the oxygenated compounds, increasing the H/C ratio, resulting in excellent stability of bio-oil-containing compounds with increased heating value and energy density.

The reaction mechanism of hydrodeoxygenation is generally described by the adsorption of the oxygenate molecule onto the catalyst surface, followed by the hydrogenation of the oxygen-containing functional group such as -OH, -COOH, or -C=O. These steps are followed by hydrogenolysis and dehydration, leading to the elimination of oxygen atoms and the formation of hydrocarbon products. Heterogeneous catalysts are crucial in hydrodeoxygenation reactions, as they reinforce the removal of oxygen atoms from oxygenate compounds and promote C-C bond formation, resulting in the production of hydrocarbons (C_xH_y) [4]. It is widely accepted that bifunctional low cost Ni-based catalysts are required; where metal nanoparticles are responsible for the H_2 transfer reactions, and the acidic sites of the support favor adsorption and activation of bio-oil compounds. Furthermore, it has recently been suggested that the deoxygenation reaction occurs at the interface between the metal and the support [5]. Thus, the role of support in the reaction mechanism remains under debate, and the development of an efficient catalyst is fundamental for the development of hydrodeoxygenation technology.

Due to the complexity of bio-oil composition, several research studies have focused on the use of model molecules representative of different fractions of bio-oil (e.g., phenol, m-cresol, anisole, and guaiacol). In this work, we prepared a series of 5% Ni catalysts supported on mesoporous sol-gel doped ZrO_2 supports with a tailored pore structure, to achieve improved metal dispersion. The Ni was added via wet impregnation technique, reduced directly in-situ whereas their catalytic activity was evaluated for the hydrodeoxygenation of acetone and phenol using different reaction conditions.

Materials and methods

The catalytic performance was investigated using resource-efficient and sustainable metal oxide catalysts in a fixed-bed Autoclave BTRS Jr. reactor. The effect of reaction conditions was evaluated by varying the temperature (200 - 400°C), liquid hourly space velocity (LHSV = 1 - 4 h^{-1}), and H_2/feed ratio (500 - 2000:1). Model bio-oil compounds (e.g., acetone and/or phenol) were used as representative feedstock components to evaluate catalyst activity, selectivity, and stability. Finally, liquid products were analyzed



off-line by gas chromatography coupled with mass spectrometry (GC-MS), while gaseous products were monitored on-line using a gas chromatograph equipped with thermal conductivity (TCD) and flame ionization (FID) detectors.

Conclusions

Bio-oil upgrading via catalytic hydrodeoxygenation reaction represents a key pathway toward sustainable liquid biofuels. Efficient deoxygenation improves fuel stability, heating value and energy density, but catalyst deactivation and the use of critical raw materials remain major challenges. In this study, different reaction conditions were employed to enhance activity, selectivity and stability, minimizing coke formation.

Acknowledgements

This research was funded in the frame of the project "Upgrading of Bio-oil over Resource-Efficient Sustainable Catalysts towards a CO_2 - neutral Economy (Acronym: SustainableCat4Fuel)", which was supported by the 4th Call of Hellenic Foundation of Research and Innovation (H.F.R.I.) Research Projects for the support of Post-doctoral Researchers (fellowship of Dr. G. Siakavelas).

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UPGRADING OF BIOMASS-DERIVED BIO-OIL TO GASOLINE AND DIESEL-RANGE HYDROCARBONS OVER RESOURCE - EFFICIENT SUSTAINABLE CATALYSTS VIA CATALYTIC CRACKING AND HYDRODEOXYGENATION: INNOVATION AND PROSPECTS - (C113)

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Keywords: Biomass-derived bio-oil, upgrading, Hydrodeoxygenation, Heterogeneous catalysis

Background and motivation

Non-renewable fossil resources like natural gas, petroleum, and coal have been the primary sources of energy and chemicals for centuries. However, their depletion and significant environmental impact create an urgent need for clean and renewable alternatives. Renewable fuels from biomass can contribute to the development of a carbon neutral economy, as they are produced in a relatively short cycle and exhibit substantially lower emissions compared to conventional diesel (no greenhouse gas emissions, no SOx emissions and 50% reduction in NOx emissions compared to conventional diesel). Up to the present moment, first generation biofuels (e.g., biodiesel) are produced from food-based biomass; however, their energy density per unit land is low and competition with food globally is a constraint. Among biomass valorization routes, cellulose and hemicellulose have been efficiently converted into liquid fuel and chemicals through hydrolysis process and subsequent treatment technologies, while lignin has typically been discarded as waste due to its poor heating value and low hydrocarbon content [1]. Currently, catalytic fast pyrolysis is the most advanced method to convert lignin into bio-oil, which can be further upgraded via the hydrodeoxygenation (HDO) process into advanced fuels (bio-gasoline and/or diesel range compounds) [2]. HDO process is necessary, as bio-oil differs from conventional diesel, i.e., raw bio-oil contains 10-40 wt.% oxygen which affects its polarity, heating values, viscosity and acidity, whereas during its storage further chemical reactions may occur (e.g. polymerization of olefins) that will deteriorate its characteristics. Along with increased moisture content (15–30%), the heating value of bio-oil (≈17-24 MJ/kg) almost half that of the commercial diesel (≈42-46 MJ/kg), decreasing its potential for utilization. Therefore, bio-oil cannot be extensively used as an energy source in current industrial and/or laboratory practices and its valorization as raw material is necessary and quite challenging.

There are two main routes to deoxygenate bio-oil: (a) catalytic cracking, and catalytic hydrodeoxygenation. The first can be performed at high reaction temperatures (400-500ºC), using acidic zeolites as catalysts, leading to the production of large quantities of coke (>20%) and reducing the yield of the desirable biofuels. Because of this, most research studies have focused on the field of the hydrodeoxygenation reaction. This process can be performed under a H_2-rich atmosphere, moderate pressure (10-30 bar), reaction temperature (250-400ºC) using selective and stable heterogenous catalysts to remove oxygen from the oxygenated compounds, increasing the H/C ratio, resulting in an excellent stability of bio-oil-containing compounds with increased heating value and energy density. It is noted that model compounds with high carbon atom number model compounds (e.g. phenol, m-cresol and/or guaiacol) are commonly used as feedstock to investigate the hydrodeoxygenation of bio-oil.

Results and discussion

This review summarizes representative studies that utilized model compounds using noble- or transition metal-based systems, bifunctional, and zeolite-based catalysts. He et al. [3] investigated the hydrodeoxygenation of guaiacol over Pt/TiO_2 catalysts promoted with Mg and Mo. They examined the effect of these promoters on catalytic performance and investigated their distinct promotion mechanisms. Specifically, Mo was found to influence Pt dispersion by modifying Pt particle size, while Mg reduced the acidity and suppressed the hydrolysis reaction path of the catalyst. These effects played a crucial role in enhancing the conversion rate of guaiacol toward fully deoxygenated cycloalkane products. In a similar process, Yu et al. [4] evaluated the catalytic



performance of Ni phosphide (P) catalysts supported on SiO_2 and HZSM-5 using phenolic compounds as feed, showing superior performance compared to Al_2O_3-supported Ni. Among them, Ni_3P exhibited the highest hydrogenation activity, while Ni_3P/HZSM-5 achieved increased HDO performance due to the bifunctional synergy between Ni_3P hydrogenation sites and the acidic dehydration sites of HZSM-5. Finally, the authors mentioned that the strong acidity of HZSM-5 further promoted cycloalkane isomerization at elevated temperatures.

Conclusions

Hydrodeoxygenation of lignin-derived model compounds is a promising route for bio-oil upgrading to produce renewable diesel and gasoline. Catalyst performance strongly depends on metal–support synergy and acidity. However, catalyst deactivation and material sustainability remain key challenges, highlighting the need for stable and resource-efficient catalyst design.

Acknowledgements

This research was funded in the frame of the project "Upgrading of Bio-oil over Resource-Efficient Sustainable Catalysts towards a CO_2 - neutral Economy (Acronym: SustainableCat4Fuel)", which was supported by the 4th Call of Hellenic Foundation of Research and Innovation (H.F.R.I.) Research Projects for the support of Post-doctoral Researchers (fellowship of Dr. G. Siakavelas).

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SUSTAINABLE PRODUCTION OF BIO-BASED GRAPHITE FOR LITHIUM-ION BATTERIES - (C117)

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Keywords: graphite, graphitization, sustainable, lignin, battery.

Abstract

Graphite remains the dominant anode material in lithium-ion batteries (LIBs) due to its structural stability, high electrical conductivity, and excellent cycling reversibility. Nevertheless, conventional graphite production relies heavily on energy-intensive processes and geographically concentrated resources, creating sustainability and supply-chain challenges. Developing renewable and locally sourced alternatives is therefore critical for strengthening material security and reducing environmental impact.

Lignin, the second most abundant natural polymer, represents an attractive bio-based carbon precursor owing to its high fixed-carbon content and aromatic structure. However, converting lignin into highly ordered graphite suitable for LIB applications remains technically challenging. In this study, lignin was fractionated in a refinery approach to obtain well-defined fractions based on physicochemical properties, which were subsequently used as precursors for bio-based graphite production.

Two graphitization strategies were investigated: catalytic graphitization and electrochemical graphitization. For catalytic graphitization, different iron-based catalysts were applied using both wet impregnation and dry mixing methods. Structural characterization revealed a strong dependence of graphitization degree on both lignin properties and processing conditions. Overall, wet impregnation with metal salts proved more effective than dry methods based on metallic or oxide particles, leading to higher structural ordering and improved graphitic characteristics. These findings highlight the importance of precursor selection and catalyst introduction strategy in advancing lignin-derived graphite for sustainable LIB anodes.

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ATMOSPHERIC PLASMA JET SYNTHESIS OF AG/TIO₂ PHOTOCATALYSTS FOR HYDROGEN PRODUCTION AND PHARMACEUTICAL POLLUTANT DEGRADATION - (C118)

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Keywords: Plasma Jet Synthesis, Ag/TiO_2 Photocatalysts, Photocatalytic Hydrogen Production, Carbamazepine Degradation,Non-Thermal Plasma (DBD)

1. Introduction

The development of integrated technologies capable of coupling renewable hydrogen production with the abatement of persistent organic pollutants is a key challenge in sustainable energy and water treatment systems. Among emerging strategies, the combination of photocatalysis with non-thermal plasma (NTP) represents a promising route to enhance reaction efficiencies while reducing energy inputs and avoiding harsh operating conditions. In this work, we investigate a dual-process approach based on the synthesis of Ag/TiO_2 photocatalysts through an atmospheric-pressure plasma jet and the simultaneous photocatalytic hydrogen evolution from aqueous carbamazepine (CBZ) solutions and CBZ degradation assisted by a dielectric barrier discharge (DBD) reactor.

2. Materials and Methods

Silver–titania photocatalysts were prepared by exposing commercial TiO_2 powders to a plasma jet operating under controlled Ar/O_2/Ag precursor flows. This method enabled the rapid deposition and reduction of Ag species onto the TiO_2 surface without the need for high-temperature treatments or chemical reducing agents, resulting in materials with improved visible-light absorption and electron–hole separation. Different Ag load were investigated. The physicochemical properties of the synthesized catalysts were characterized through XRD, UV–Vis DRS, Raman, and BET analyses, to confirm the formation of Ag nanoparticles and the preservation of TiO_2 crystallinity.

Photocatalytic hydrogen evolution tests were carried out in a custom batch Pyrex reactor (inner diameter 2.5 cm, height 18 cm) operated at atmospheric pressure and room temperature. A constant N_2 flow (250 $Ncm^3\ min^{-1}$), controlled by a mass flow controller, was used to purge the system before irradiation, maintain inert conditions, and transport evolved gases to the analytical unit. The reaction mixture consisted of an aqueous carbamazepine solution (10 ppm) with a total volume of 80 mL, in which the photocatalyst was dispersed at loadings between 0.5 and 2 g L^{-1}. A peristaltic pump ensured continuous recirculation and homogeneous dispersion. Before irradiation, the suspension was kept in the dark for 60 min to allow adsorption–desorption equilibration.

Photocatalytic reactions were performed under visible light for up to 240 min using four 8 W Philips lamps positioned symmetrically around the reactor (emission range 400–700 nm). The evolved gases were monitored online using an ABB Advance Optima analyser equipped with a thermal conductivity detector (CALDOS). Gas concentration data were collected in real time via LabVIEW and processed in Origin. The degradation experiments for carbamazepine were carried out in a cylindrical dielectric barrier discharge (DBD) reactor. The reactor was inclined at 30° to ensure a uniform wastewater flow through the quartz tube. The system consisted of two coaxial quartz tubes: the inner tube (9 mm i.d., 1.5 mm wall) housed an 8 mm diameter copper high-voltage electrode, while the outer tube (200 mm length, 24 mm i.d., 1.5 mm wall) was wrapped with a stainless-steel mesh acting as the grounded electrode (90 mm active length). Plasma was generated in the discharge gap between the electrodes, separated by the quartz dielectric, forming the DBD configuration. The carbamazepine degradation was monitored through spectrophotometric analysis coupled with HPLC-MS.



3. Results and Discussion

The Ag/TiO_2 catalysts exhibited superior H_2 generation compared to bare TiO_2, attributable to plasmon-induced charge separation and improved surface reactivity. In parallel, the DBD non-thermal plasma system enabled the generation of reactive oxygen and nitrogen species (RONS), which contributed to the degradation of CBZ, facilitating its mineralization and reducing the formation of recalcitrant byproducts.

4. Conclusions

Coupling the plasma-assisted catalyst synthesis with a hybrid photocatalysis–NTP treatment demonstrated the potential for an integrated and energy-efficient approach for simultaneous renewable fuel generation and pollutant removal. The synergy between photocatalysis and plasma processes enhanced both hydrogen production and CBZ degradation, suggesting promising applicability in wastewater-to-energy conversion frameworks. This study provides novel insights into the role of plasma technologies in the design of advanced photocatalysts and in the development of sustainable multifunctional treatment systems.

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INFLUENCE OF ALKALI METAL PROMOTION (K, NA, CS) ON SELECTIVITY AND PRODUCTIVITY OF CUFEZN/M-ZRO₂ CATALYSTS IN CO2 HYDROGENATION - (C119)

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Keywords: CO_2 hydrogenation; Multifunctional catalyst; Higher alcohols; Olefins

1. Introduction

The catalytic hydrogenation of CO_2 to produce higher alcohols and olefins, compounds with wide use in industry and applications such as fuels, has attracted great research interest[1,2]. The main challenge for this process is the coupling of the C-C bond, due to the stability and chemical inertness of CO_2. Herein, catalysts were synthesized and tested by combining the CuZn, known for the production of methanol, with the Fe, a metal responsible for the propagation of carbon chain through the formation of C-C bonds while ZrO_2 was utilized as the support. In addition, the effect of different alkali metal (K, Na and Cs) on the catalytic activity of a CuFeZn/ZrO_2 catalyst was investigated towards maximizing the selectivity and yield of higher alcohols and olefins.

2. Materials and Methods

The different alkali promoted CuFeZn supported on ZrO_2 catalysts were prepared via the wet impregnation method achieving a total metal loading of Cu, Fe, Zn equal to 30 wt% (with a molar ratio of 1:2:1) and a K, Na or Cs loading of 3 wt%. The catalytic experiments were carried out in a fixed-bed reactor using T= 320 °C, P= 30 bar and WHSV= 12000 mL g^{-1} h^{-1}. Prior to the reaction the catalysts were reduced at 400 °C for 1h at atmospheric pressure. All the catalysts were characterized by N_2-physisorption, H_2-TPR and CO_2-TPD.

3. Results and Discussion

At 320 °C (P = 30 bar, H_2/CO_2 = 3, WHSV = 12,000 mL·g^{-1}·h^{-1}), the nature of the alkali has a decisive influence on both the selectivity and the space-time yield (STY) of the catalyst CuFeZnO(1:2:1)/m-ZrO_2. As shown in Figure 1, the Na-promoted catalyst exhibits the maximum total selectivity to olefins and higher alcohols and the highest STY, which indicates the most favorable combination of selectivity and activity among the alkali examined.

In contrast, modification with K leads to lower olefin selectivity while the use of Cs visibly shifts the product mix towards more hydrogenated compounds, with increased paraffins and methane and significant suppression of olefins, higher alcohols and the C_{5+} fraction. The observed trends indicate that the role of alkali is not simply limited to increasing surface basicity, but is related to the regulation of electron structure, surface hydrogen chemistry, and the active phase of Fe. In the present system, Na appears to offer an optimal level of modification, sufficient to enhance CO_2 activation and limit the secondary hydrogenation of olefin intermediates, without causing intense blockage of active sites or excessive hydrogenation, as observed in the case of Cs. The stabilization and functionality of iron carbides (FeCx), which are widely considered to be the active phases for C–C coupling and chain development in Fe catalysts for the hydrogenation of CO_2 played a decisive role in the increased olefin selectivity of the sample with Na. Also, promotion with Na has been reported to facilitate the formation of FeCx and protect them against oxidation by the produced H_2O (a product of RWGS), maintaining a high probability of increasing the carbon chain and producing olefins. In contrast, in the case of Cs, stronger electron donation activity and larger ionic size can limit the functionality of FeC_x through modification of surface



hydrogen coverage, favoring the hydrogenation of intermediate species and leading to increased selectivity towards paraffins and methane.

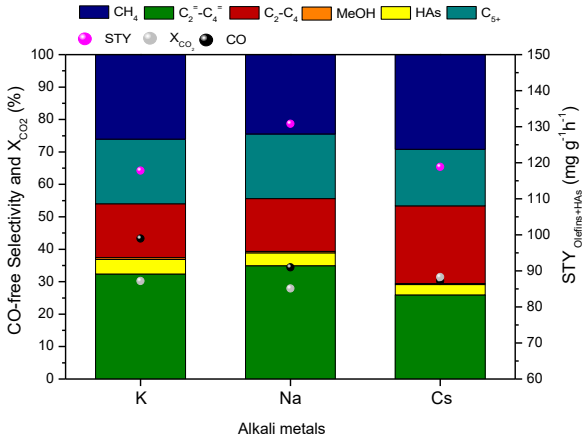


Figure 1. Effect of different alkali metal (3wt%) on the catalytic activity of the catalyst CuFeZnO(1:2:1)/m-ZrO_2. Reaction conditions: T= 320 ºC, P= 30 bar, H_2/CO_2= 3, WHSV= 12,000 $mLg^{-1}h^{-1}$.

4. Conclusions

Overall, the results demonstrate that Na is the optimal alkaline modifier for the catalyst CuFeZnO/m-ZrO_2 under the present reaction conditions, while achieving the highest selectivity towards olefins/alcohols and maximum productivity among the alkalis, through balanced electronic modification, favorable regulation of surface hydrogen chemistry and effective stabilization of the active carbide phase of Fe.

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DESIGN AND SIZING OF A DEMONSTRATION PLANT FOR THE ANALYSIS OF THE SUMMER SOLAR DESORPTION PROCESS IN AN OPEN-CYCLE THERMOCHEMICAL SEASONAL STORAGE SYSTEM - (C142)

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Keywords: Termo-chemical storage, Seasonal heat storage, Solar thermal energy

1. Introduction

Seasonal Thermo-chemical Heat Storage (sTCHS) is a promising route to increase the solar fraction of space heating by decoupling energy collection and demand over long time scales. In terms of plant layout, the open-cycle TCHS configuration can use ambient water vapor from domestic activities and avoids deep-vacuum evaporators/condensers, enabling simpler and potentially cheaper architectures for residential applications. A separated-reactor configuration instead decouples the reactor from long-term storage tanks, allowing a compact unit near the user and remote sorbent storage, improving integration and system flexibility. The optimal direct coupling between the reactor and solar collectors is crucial, as regeneration conditions and process control strongly affect the effective energy density of the thermochemical material. In this work, a detailed analysis of possible system configurations and operational constraints for the summer charging-stage of a TCHS will be presented. In the following project step, the same plant configuration will be constructed and tested. The solar desorption demonstration plant will be employed to test and evaluate the performance of the summer charging phase for the seasonal storage cycle in a variety of conditions.

2. Methods

Firstly, a review of existing thermal solar collectors' technologies has been conducted through a systematic analysis of public databases (especially the Solar Keymark [1] database) and information available on the web. The thermal efficiency curves of the solar collectors have been compared to the desorption temperatures employed in the open-cycle TCHS systems found in the literature, ranging between 120 – 220 °C. Then, the suitable solar collectors have been analyzed in terms of annual energy productivity for a reference location (Milan, Italy), with the goal of identifying the technology with the highest energy yield. The actual solar desorption plant configuration has been defined based on the technological constraints of a hypothetical domestic application; the system will employ a batch-operated, separate-reactor configuration with an auger reactor to minimize the thermal inertia and react readily to oscillations of solar energy availability. Lastly, a simplified numerical model of the reactor has been exploited to optimize the geometrical features of the reactor in order to maximize the usage of solar energy.

3. Results, Discussion and Conclusions

The survey of thermal solar collectors has shown that Compound Parabolic Collectors (CPC) would provide an optimal conversion of solar radiation to exploitable thermal energy for the specific location and typical open-cycle thermochemical storage desorption temperatures. The identified plant configuration will involve a solar thermal loop that exploits a liquid heat transfer fluid (ideally thermal oil) to heat the desorption air up to 220 °C. The plant will also include an air-air heat recovery exchanger to minimize the



energy losses. The reactor will be an auger-type, counter-flow screw vessel, operated with stepwise feed of thermochemical material that will be progressively dehydrated by the incoming air stream.

One of the key points of the system design is the definition of the geometrical features of the reactor. A numerical model has been developed to evaluate the detailed dynamic behavior of the system; the model is based on a previous architecture representing a packed-bed adsorption column filled with Zeolite 13X [2]. The parametric simulations of a typical desorption test have been carried out by defining a reference condition in terms of solar irradiation (600 W/m^2), solar collectors surface area (10 m^2), ambient temperature (20 °C), and humidity (5 g_V/kg_A). The parametric simulations have been evaluated in terms of a specific performance index, called Regeneration Index (IR), that combines solar conversion efficiency with the reactor's energy efficiency (Figure 38). The results have shown that the optimal reactors aspect ratio (L/D) is equal to 6, while the sorbent mass contained in the vessel should be limited to 1 kg. These numerical results will be used to design the demonstration plant that will be built in the next phase of the project.

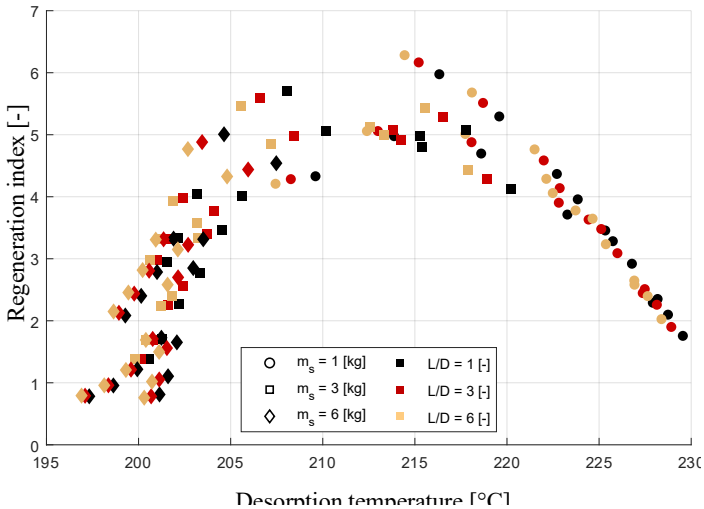


Figure 38: Trend of the regeneration performance index for different geometrical features of the reactor.

Acknowledgements

This work has been financed by the Research Fund for the Italian electrical System under the Three-Year Research Plan 2025-2027 (MASE, Decree n.388 of November 6th, 2024), in compliance with the Decree of April 12th, 2024.

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SULFONATED POLYSULFONE AND NANOCOMPOSITE POLYMER ELECTROLYTE MEMBRANES FOR ADVANCED POWER DEVICES - (C144)

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The development of cost-effective proton exchange membranes (PEMs) as an alternative to traditional Nafion and other perfluorosulfonic acid (PFSA) membranes is crucial for the implementation of advanced electrochemical energy technologies. Such materials are particularly interesting for green hydrogen applications, such as Proton Exchange Membrane Fuel Cells, Polymer Electrolyte Membrane Water Electrolysers, and solid-state energy storage devices.

This study focuses on alternative fluorine-free polymer electrolyte membranes based on sulfonated polysulfone (sPSf), which were synthesised and thoroughly investigated. The sPSf polymer was synthesised using a mild and sustainable homogeneous sulfonation procedure using the trimethylsilyl chlorosulfonate as the sulfonating agent. Additionally, at the preparation of pristine sPSf polymer, other nanocomposite membranes were prepared by incorporating silica and sulfonated silica (SiO_2) nanoparticles into the sulfonated polymer matrix to enhance the physicochemical properties and electrochemical performance of the membranes.

All of the prepared PEMs were characterised using several physicochemical techniques, including thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) and Raman spectroscopy. Additionally, ion exchange capacity (IEC), water uptake and the hydration number (λ) were used to assess hydration behaviour and proton and sodium ion conductivity of the membranes.

Due to time constraints, the electrochemical characterisations of the developed membranes were evaluated preliminarily in neutral aqueous environments (pH around 7) in solid-state supercapacitor configurations. These initial studies provide insights into ionic transport and conductivity features and can help to assess the electrochemical stability window of the membranes up to 2 volts, as is the case with solid-state supercapacitors. Comprehensive analysis using ATR-FTIR and Raman, combined with thermal and electrochemical characterisations, reveals that the synthesised sPSf polymer and its nanocomposites demonstrate occurred sulfonation, with adequate ion exchange capacity (1.34 $meq \cdot g^{-1}$) and high ionic conductivity (≈3-5 $mS \cdot cm^{-1}$). They also demonstrate comparable, or even superior, capacitance metrics to those of commercial PFSA-equivalent membranes. Future investigations will focus on testing these materials under more stringent pH acid conditions, initially in PEM water electrolysers and then in PEM fuel cells.

Acknowledgments

The authors of CNR-ITAE thanks the European Union – Next Generation EU from the Italian Ministry of Environment and Energy Security POR H2AdP MMES/ENEA with involvement of CNR and RSE, PNRR -Mission 2, Component 2, Investimento 3.5, CUP B93C22000630006 "Ricerca e sviluppo sull'idrogeno".

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THERMO-FLUID DYNAMIC ANALYSIS OF THE AIR PRE-HEATHER FOR A SOFC SYSTEM FED BY AMMONIA - (C148)

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Keywords: Air pre-heater design, 3D stationary modeling, Thermo-fluid dynamic analysis, CFD, SOFC system

1. Introduction

Solid Oxide Fuel Cells (SOFCs) are pivotal for high-efficiency power generation, yet their high operating temperatures demand precise thermal management. Pre-heating oxidant air is critical to prevent catastrophic thermal gradients within the ceramic stack. While current literature often relies on simplified 0D/1D lumped parameter models in complex SOFC systems fed by syngas or biogas [1,2] or on more complex models of simpler planar geometries [3] to reduce computational costs, these overlook complex local heat transfer effects in more complex geometries. This work addresses this gap by developing a 3D stationary thermo-fluid dynamic model based on the actual, intricate geometry of a real pre-heat exchanger in Comsol Multiphysics 6.2 calculation environment. By capturing local turbulence and temperature distributions, this study provides a novel, high-fidelity tool for robust SOFC system integration.

2. Materials and Methods

The 3D stationary model was built in COMSOL Multiphysics® 6.2 using the Turbulent Flow, Heat Transfer in solids and fluids and Non-Isothermal Flow coupled modules. The real geometry was discretized with a fine physics-controlled mesh, refined at wall boundaries. Steady-state Navier-Stokes and energy equations for a turbulent flow with k-e model were solved to couple fluid flow and heat transfer. Results were processed via 3D volume plots to analyze the temperature maps inside the main pre-heater solid components and in the air along the helical tube and the air pressure drops in the helical tube, validating the heat exchanger's effectiveness and fluid distribution.

3. Results and Discussion

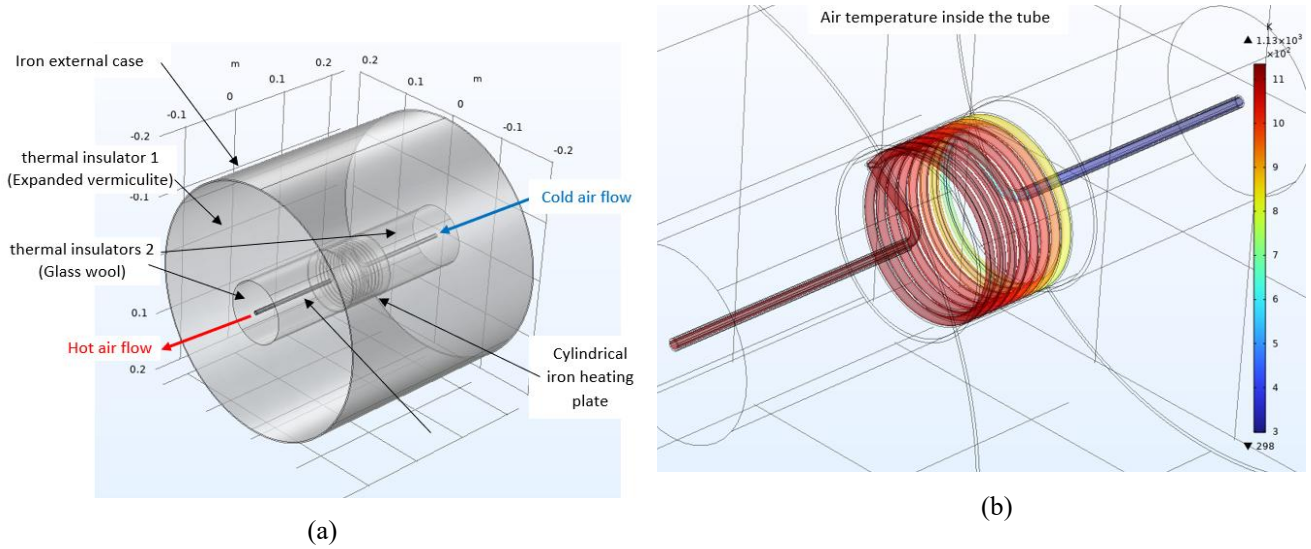
The air pre-heat exchanger geometry, component and materials are shown in Figure 1(a). The pre-heater is mainly composed of a helical 8-turn iron tube, in which the air to be heated flows, of a cylindrical iron heating plate, two cylindrical elements of a first thermal insulator in glass wool, a cylindrical element of a second thermal insulator in expanded vermiculite and an external iron case. Figure 1(a) also shows the pre-heater's external dimensions.

Table 1 shows the values of the main input parameters. For the sake of brevity in figure 1(b) only the air map temperature inside the helical tube is shown and in the steady state condition and at maximum output thermal power of the cylindrical heating plate the air temperature at the pre-heater outlet is about 1130 K and it is compatible with the SOFC stack maximum operating temperature of 1123.15 K, therefore the designed air pre-heater performs its function correctly.

Table 2 Main input parameters

Input parameter	**Unit**	**Value**
Inlet air temperature, $T_{in,air}$	K	298.15
Inlet air flow, $Q_{in,air}$	m^3h^{-1}	10
Tube internal diameter, $D_{in,tube}$	cm	0.46
Tube thickness, t_{tube}	mm	0.9
Maximum output thermal power of the cylindrical heating plate, $P_{th,out,hp}$	kW	3





(a) (b)

Figure 1 Air pre-heat exchanger geometry, component and materials (a) and trend of air temperature inside helical tube (b)

4. Conclusions

In this work, a calculation tool was set up in the COMSOL Multiphysics 6.2 environment for the verification and design of the pre-heater for the air at the inlet of an ammonia-fueled SOFC system. It is capable of evaluating the temperature maps of all the main solid components of the preheater and the pressure and temperature maps of the air inside the preheater operating under steady-state conditions. The results obtained showed that the designed air pre-heater performs its function correctly.

Acknowledgements

This research was funded by the European Union – NextGeneration EU from the Italian Ministry of Environment and Energy Security POR H2 AdP MMES/ENEA with involvement of CNR and RSE, PNRR - Mission 2, Component 2, Investment 3.5 “Ricerca e sviluppo sull’idrogeno”

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PRESSURISATION STRATEGIES FOR SOLID OXIDE ELECTROLYSIS CELLS: A COMPARATIVE OVERVIEW - (C156)

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Keywords: SOEC, Electrolysis, Pressurisation, Hydrogen Production

1. Introduction

Solid Oxide Electrolysis Cells (SOECs) are a promising technology for high-efficiency hydrogen production. However, pressurisation results in design challenges and increased costs. This work proposes a comparison between different pressurisation strategies for SOECs systems. Three pressurisation technologies were identified: Hot Box Vessel (HBV) pressurisation; Post-Compression (PC) and Vessel-free Differential Pressurisation (VFDP). Trade-offs in efficiency, system integration, mechanical sealing and thermal management are discussed. Direct stack pressurisation improves system efficiency by reducing compression losses. However, the chosen pressurisation technology is the trade-off between performance benefits against capital cost, heat losses, and pressure-control challenges.

2. Materials and Methods

A systematic literature review was carried out for this work. Peer-reviewed studies were grouped according to the different pressurisation strategies, i.e., Hot Box Vessel pressurisation; Post-Compression and Vessel-free Differential Pressurisation. Technologies were compared in regard to operating pressure, system efficiency, costs, design complexity, and thermal management, allowing identification of current design strategies and trade-offs.

3. Results and Discussion

Research revealed that pressurised SOECs have higher system efficiency than their atmospheric counterpart [1]. Three technological solutions for SOECs pressurisation have emerged from the literature:

- Hot Box Vessel (HBV) pressurisation - direct stack pressurisation within insulated hot box
- Post-compression (PC) systems - mechanical compression following atmospheric electrolysis
- Vessel-free differential pressurization (VFDP) - upstream fuel-side pressurization

In the HBV configuration, the SOEC stack is kept under pressure within a vessel filled with an inert gas. The technology allows for pressure operations up to 15 bar and high steam conversion [2]. Main advantages include good system integration and higher efficiencies due to reduced compression energy needs in comparison to the post-compression design. Limitations involve added CAPEX from vessels cost and increased heat losses. The challenges mainly consist in reducing differential pressure to prevent cells' cracking and leaks and reducing thermal losses to the surrounding.

PC solutions enable H_2 compression downstream of the atmospheric electrolyser. However, energy-intensive compressors are required for gas compression. This simplify the stack design and allows easier maintenance, while the main limitation is the extra work required for gas compression (efficiency reduced by 5%) [3]. In VFDP technology, upstream fuel-side pressurisation achieves differential pressure using manifold designs to pressurise the reactant side. This configuration typically achieves high system efficiencies. However, the technology is limited to lower pressure ratios due to sealing risks, potential cross-leakage, and mechanical stress from pressure differentials. Table 1 provides a comparative overview of the pressurisation technologies used in SOECs.



Overall, the literature suggests that pressurisation improves SOEC performance, but the best configuration depends on the target pressure, plant scale, and budget costs.

Table 3: Comparative overview of the three compression technologies used in SOECs

Parameter	Vessel-Free (Differential)	Hot Box Vessel	Post-Compression
Operating Pressure	Few bars Differential pressure	10-25 bar	1 bar +30 bar final
System Efficiency	High, but design-dependent	High	Lower due to compression penalty
Capital Cost (CAPEX)	Moderate	High	Low (stack) - High (compressor)
Operational Cost (OPEX)	Low	Moderate	High
Sealing Complexity	High	Moderate	Low
Thermal Losses	Minimal	High	Minimal
Main Benefit	Avoids vessels while retaining pressurisation benefit	Good integration with high-pressure process trains	Simple Stack Architecture

4.Conclusions

The study investigated the design characteristics of current SOEC solutions, focusing on comparing pressurization strategies found in literature. Direct stack pressurization improves overall efficiency by reducing downstream compression requirements, nevertheless sealing risks and mechanical stress on components must be addressed. PC solutions simplify the stack design but result in higher pumping losses. Consequently, current technological choices hinge on balancing system performance with application-specific costs.

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ELECTROCHEMICAL WATER OXIDATION FOR IN-ORBIT H_2O_2 PRODUCTION: TRL-4 VALIDATION IN A FLOW-CELL REACTOR - (C158)

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Keywords: green propellants, H_2 production, H_2O_2 production, PV-EC system, $2e^-$ water oxidation reaction

1. Introduction

Water is a key resource for long-term space operations. It is non-toxic, relatively abundant on many planetary bodies and can serve multiple roles simultaneously: a life-support fluid, radiation shielding, thermal mass, and a feedstock for propellant production. The Green SWaP (Green Solar-to-propellant Water Propulsion) project leverages water as a strategic in-space resource to build an integrated ecosystem that couples solar-to-propellant conversion with advanced storage and propulsion technologies, enabling the sunlight-driven production of H_2O_2 and H_2 for a practical bimodal system that bridges the performance gap between chemical and electric propulsion across diverse mission profiles. Here we present some of the activities developed within the PV-EC approach for H_2O_2 and H_2 production, aimed at building and validating, at the TRL-4, a flow cell reactor system.

2. Materials and Methods

A preliminary Front-End Engineering Design (FEED) evaluation was carried out considering piping and reactor components compatibility for concurrently production of H_2O_2 and H_2 in a paired electrochemical flow-cell. The idea of this cell assembly was aimed to use water for both anode oxidation to H_2O_2 and cathode reduction to H_2 for in-orbit bipropellant production. In the preliminary test with RRDE technique screened electrocatalysts such as TiO_2 NTs[1], Degussa P25, g-C_3N_4[2], and Pd-0.3%-N-CNTs were used as anode for the $2e^-$ WOR electrosynthesis of H_2O_2 in bidistilled water, 0.1 M NaOH, and 1 M $KHCO_3$ to identify the most efficient catalyst/electrolyte combination. Whereas Ni_3N/Ni as cathode for water reduction to H_2 in alkaline electrolyte will be used. Once the catalyst/electrolyte system has been selected and tested in a lab-scale electrocatalytic device (size electrodes ~10 cm^2) operating at room temperature in flow conditions, the work will be focused on the engineering and optimization of a continuous-flow PV-EC reactor.

3. Results and Discussion

The procurement and assembly of the components allowed for the creation of a stable configuration for continuous operation, ensuring controlled electrolyte flow and the simultaneous production of H_2O_2 at the anode and H_2 at the cathode (Figure 1). The reactor consists of anode and cathode compartments separated by a FUMASEP anion exchange membrane (AEM) and fed via independent anolyte and catholyte recirculation circuits to limit product crossover, while an Ag/AgCl reference electrode positioned close to the anode allowed for precise potential control while minimizing ohmic losses. Integration with a silicon heterojunction (SHJ) photovoltaic module will follow, allowing the system to operate directly without external power supplies. Coupling the PV-EC device requires parameter optimization to balance the PV module's maximum power point with the cell's electrochemical requirements, while maintaining catalyst operation within their stability window. The test campaign will be carried out by powering it with a Metrohm PGSTAT30 potentiostat/galvanostat, while the final test, after selecting the cathode and anode materials and optimizing all the electrochemical parameters, will take place by irradiating the photovoltaic panel with a solar simulator.



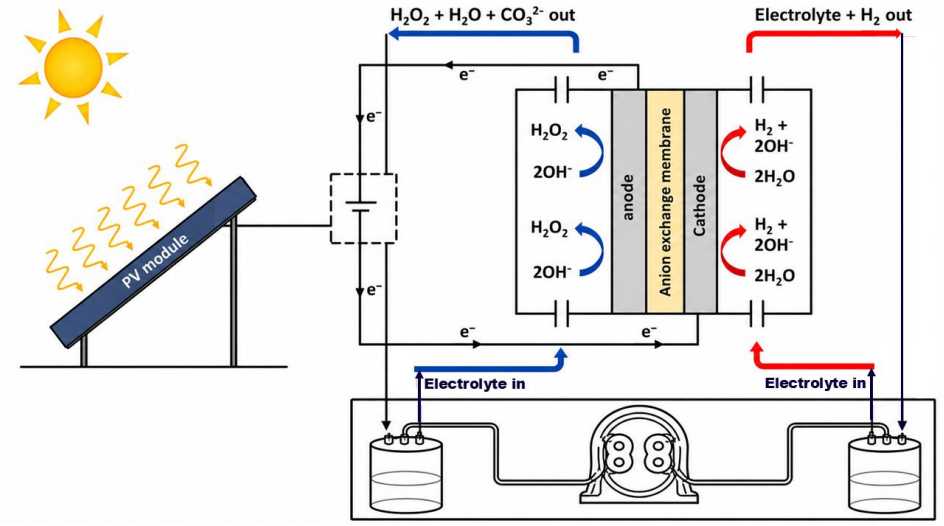


Figure 1. PV-EC reactor showing anodic and cathodic compartments separated by AEM and connected to their respective reservoirs through recirculation system driven by a peristaltic pump. The system is powered by a SHJ photovoltaic module.

4. Conclusions

The developed device demonstrates the feasibility of the simultaneous production of H_2O_2 and H_2 in a continuous-flow PV-EC configuration. The engineered flow-cell provides promising results for TRL-4 validation of the system and represents a significant step toward the development of integrated water-to-propellant technologies for future in-space applications.

Acknowledgements

This work was supported by the HORIZON EIC Grants under the Green SWaP project, ID 101161583.

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ELECTROCHEMICAL WATER OXIDATION FOR IN-ORBIT H_2O_2 PRODUCTION: INSIGHTS ON MECHANISM FROM RRDE ANALYSIS - (C159)

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Keywords: $2e^-$ water oxidation reaction; electrochemical H_2O_2 production, in-situ H_2O_2 quantification, RRDE analysis, green propellants

1. Introduction

The electrochemical two-electron water oxidation reaction[1] ($2e^-$ WOR) has been investigated as a promising route for the decentralized production of H_2O_2. This research is central to the Green Solar-to-propellant Water Propulsion (Green SWaP) project, which aims to establish a sustainable method for producing bi-propellants (H_2O_2/H_2) directly in space. This approach enables sustainability of future space missions, facilitating safer and more efficient in-orbit services. Accurate detection of H_2O_2 in real time production is critical for evaluating electrocatalysts selectivity in $2e^-$ WOR. Herein, the performance of titanium- & carbon-based electrocatalysts were investigated using RRDE for in-situ H_2O_2 production and detection. Based on the screened results, selected catalysts will be used for the development of the benchmark anode for a flow-cell device to produce green bi-propellant.

2. Materials and Methods

The catalysts (TiO_2 NTs & g-C_3N_4) were prepared according to previously described protocols[2] and deposited as ink onto a GC disc of RRDE tip (Metrohm RRDE Pt-GC tip 5 mm, 0.196 cm^2, N=24.9%). For electrochemical measurements, a thermostat three-electrode cell (25 °C, 1 atm) equipped with ink-deposited RRDE tip (ink-deposited disc WE1; Pt-ring WE2), platinum rod (CE) & Ag/AgCl (RE) was used. The electrolytes investigated were bi-distilled H_2O, 0.1 M, 0.5 M and 1 M $KHCO_3$. Hydrodynamic linear sweep voltammetry (LSV) and Chronoamperometry (CA) tests were carried out by using a Metrohm PGSTAT30 workstation.

3. Results and Discussion

The Rotating Ring-Disk Electrode (RRDE) technique offers the possibility to investigate the $2e^-$ WOR by simultaneously driving the production of H_2O_2 at the disk and detecting its oxidation at a downstream electrode (the ring) under controlled mass transport (rotation). Water is oxidized to H_2O_2 at the rotating disk (WE1) via $2e^-$ WOR. This generated H_2O_2 diffuses outward to the Pt ring (WE2), which is set at a potential suitable to oxidize H_2O_2 to O_2 and produce a ring current (I_r) that is directly proportional to the amount of H_2O_2 generated at the disk, as detailed in schematic Figure 1a. To compare the performance of the electrocatalysts in the $2e^-$ WOR, the selectivity ($FE_{H_2O_2}$) and mole fraction of produced H_2O_2 ($\chi_{H_2O_2}$) were quantified[3] as follows:

$$FE_{2e^-WOR} = \frac{|I_r|/N}{|I_d|} \times 100 \qquad \text{and} \qquad \chi_{H_2O_2} = \frac{2|I_r|/N}{|I_d|+|I_r|/N} \times 100$$

We have investigated different rotation speed to identify effective mass transport and avoid the detachment of the catalyst from the disc surface by using g-C_3N_4 in 1 M $KHCO_3$. Moreover, we observed the maximum selectivity (e.g. FE of 46.36% & χ of 63.35% at 3000 rpm) at the beginning of each rotation speed cycle due to the H_2O_2 accumulation during the transition time (~16 sec) between two successive cycles, as reported in Figure 1b. These results imply that the catalyst is promising for the $2e^-$ WOR under optimized conditions. The best selectivity results have been obtained for g-C_3N_4 in 0.5 M $KHCO_3$ with FE of 7.14% and χ of 12.97 % at 1.94 V_{RHE}, as shown in Figure 1c. These results provide real-time information for $2e^-$ WOR, enable accurate analysis of catalysts



selectivity by ensuring efficient mass transport, and make RRDE a valuable tool for screening and developing highly selective electrocatalysts.

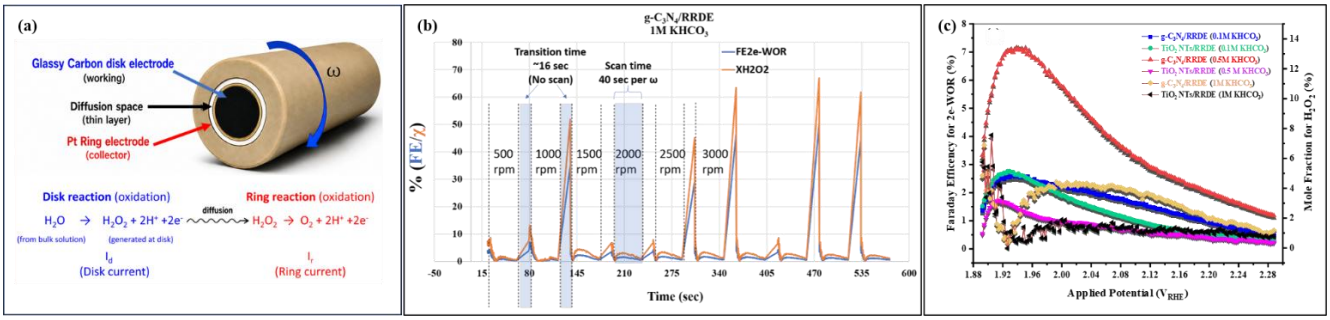


Figure 1. a) Scheme of RRDE technique for H_2O_2 production and detection. b) Calculated FE and H_2O_2 molar fraction for g-C_3N_4 in 1M $KHCO_3$ at different rotating speed. c) Selectivity of TiO_2 NTs & g-C_3N_4 in different electrolytes at 1500 rpm.

4. Conclusions

RRDE method was successfully used for evaluating electrocatalyst efficiency and mechanism, which provide direct evidence of reaction pathways and catalyst selectivity toward H_2O_2. The obtained results will be used for the development and optimization of an electrochemical system, which allows in-orbit H_2O_2 production.

Acknowledgements

This work was supported by the HORIZON EIC Grants under the Green SWaP project, ID 101161583.

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MULTIFUNCTIONAL GETESE CHALCOGENIDE AS A PROMISING ELECTRODE MATERIAL FOR ADVANCED LITHIUM-ION BATTERIES - (C162)

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Keywords: Thin films, chalcogenides, phase change material, energy-efficient.

1. Introduction

GeTeSe chalcogenide material was synthesized and comprehensively characterized to explore its potential for advanced energy-storage and memory-device applications. Structural characterization confirmed the formation of a stable phase with favourable amorphous–crystalline transition behavior, while optical studies revealed suitable electronic band-gap properties that can support charge-transfer processes. Performed thermal analysis demonstrated good thermal stability and phase-transition characteristics, which are important for maintaining electrochemical performance during repeated charge–discharge cycles in battery systems. Electrical characterization showed enhanced conductivity and significant resistance variation associated with structural transformation, indicating efficient electron transport behavior.

The unique combination of thermal stability, tunable electrical conductivity, and phase-transition capability makes GeTeSe a promising multifunctional chalcogenide material for rechargeable battery technologies, particularly in electrode and solid-state energy-storage applications where rapid ion/electron transport and structural durability are essential. In addition, the presence of Ge and Te-based chalcogenide networks may provide improved electrochemical activity and cycling stability due to their adaptable bonding structure and defect-mediated transport mechanisms, highlighting its potential as an energy-efficient material for integrated electronic and electrochemical storage technologies.

2. Materials and Methods

GeTeSe chalcogenide material was synthesized using the conventional melt-quenching technique. Thin films were deposited using thermal-evaporation technique. The structural properties of the synthesized GeTeSe material were investigated using X-ray diffraction (XRD) analysis to determine phase formation, crystallinity, and amorphous behavior. Surface morphology and elemental composition were examined using scanning electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (EDS). The obtained results confirmed the homogeneous distribution of constituent elements in the material. Optical properties of the GeTeSe material were studied using UV–Visible spectroscopy in the selected wavelength range. The absorption spectra were used to estimate the optical band gap and investigate electronic transition behavior. Thermal stability and phase-transition behavior of the synthesized material were analyzed using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). Electrical properties of the GeTeSe material were investigated using current–voltage (I–V) measurements and resistivity analysis at different temperatures.

3. Results and Discussion

The amorphous/crystalline structural adaptability of GeTeSe may provide favorable pathways for lithium-ion diffusion and reversible electrochemical reactions. The observed thermal stability of GeTeSe indicates its suitability for electrochemical systems operating under repeated charge–discharge and thermal stress conditions. The optical parameters having bandgap ~1.18eV that provides adequate electronic conductivity and structural tunability. The observed electrical response was analyzed in relation to potential applications in lithium-ion battery systems and phase-change memory devices, where efficient electron transport and thermal stability are important performance parameters. Improved charge-transfer kinetics in lithium-ion battery electrodes.



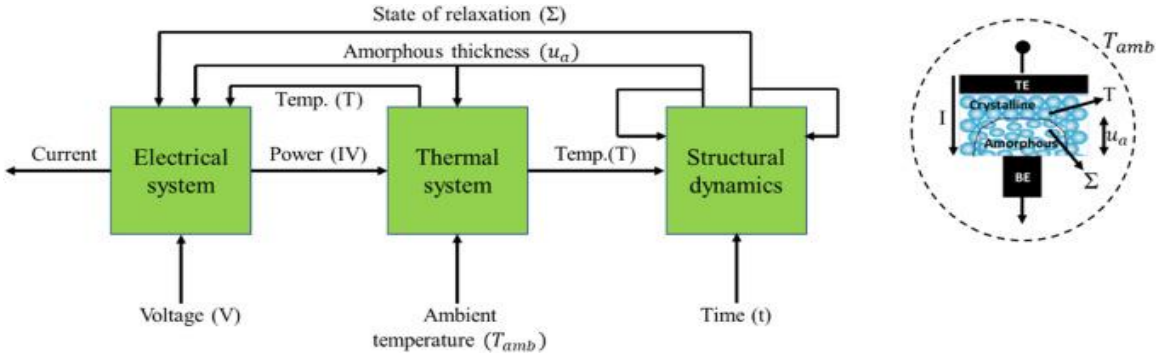


Fig. Block diagram of PCM device showing combination of electrical, thermal, and structural dynamics.

4. Conclusions

Overall, the present study highlights the potential of GeTeSe as a multifunctional material for next-generation energy-storage and memory technologies. In order to fully understand applicability of such material in devices, further electrochemical investigations, including cyclic voltammetry, charge–discharge cycling, and impedance analysis, are necessary to be performed in half and full cell configuration.

Acknowledgements

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MULTIPHYSICS FINITE ELEMENT MODELING OF ELECTRIFIED STRUCTURED CATALYSTS FOR SUSTAINABLE HYDROGEN PRODUCTION - (C170)

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Keywords: Hydrogen production, Electrification strategies, Joule heating, Structured catalysts, Multiphysics modeling

1. Introduction

Hydrogen is a key energy carrier for the transition towards a low-carbon energy system, yet its production still relies on fossil-fuel-heated reforming, causing substantial CO_2 emissions [1]. Replacing conventional external heating with electrically driven solutions represents a promising decarbonization strategy. Among these, direct Joule heating of conductive structured materials enables volumetric heat generation, reducing thermal inertia, enhancing temperature controllability, and potentially improving process efficiency [2]. However, the rational design of such systems requires a deep understanding of the coupling between electrical, thermal and fluid-dynamic phenomena within complex porous architectures. This work proposes a multiphysics finite element modeling (FEM) framework to investigate the behavior of silicon-infiltrated silicon carbide (SiSiC) structured catalysts, providing design-oriented insights for next-generation electrified hydrogen production systems.

2. Materials and Methods

A SiSiC structured support was modeled in *COMSOL Multiphysics® 5.6* by generating a fully resolved three-dimensional ordered open-cell lattice. The multiphysics framework coupled *Electric Currents*, *Heat Transfer in Solids and Fluids* and *Laminar Flow* interfaces. Joule heat generation within the solid phase was accounted for through the *Electromagnetic Heating* multiphysics, while *Nonisothermal Flow* was implemented to handle the fluid-dynamic and thermal interactions at the solid-fluid interface. Argon was used as a non-reactive flowing gas to investigate the intrinsic electro-thermal response of the structured foam without the additional complexity introduced by chemical reactions. Furthermore, to accurately simulate the experimental setup and account for realistic radial heat losses, the computational domain was extended to include the reactor wall and an external layer of glass wool insulation.

3. Results and Discussion

The SiSiC foam was selected due to its suitability for electrified reactor configurations, combining electrical conductivity, high-temperature stability, and an open-cell architecture that promotes efficient heat and mass transfer while simultaneously acting as both a structural support and a resistive heating element [3].

The simulation results, illustrated in Figure 1, describe the steady-state spatial temperature distribution within both the solid and fluid domains. Upon applying a potential difference of 2 V, volumetric Joule heating is generated within the electrically conductive matrix. As shown in Figure 1a, the SiSiC core attains a maximum temperature of approximately 531 K, with a high degree of thermal uniformity in the central heated zone. Moving radially outward (Figure 1c), a clear temperature gradient is observed as heat is dissipated toward the reactor wall and the external glass wool insulation, with the boundary temperature dropping to 312 K.

From the fluid dynamic perspective, argon is fed at the reactor inlet (bottom) at 295 K with a flow rate of 1000 NmL/min. The foam's architecture facilitates an extremely efficient solid-to-gas heat exchange, resulting in a steep axial temperature profile (Figure 1b). Along most of the reactor length, the gas remains in near-thermal equilibrium with the solid and exits the reactor at



approximately 528 K. The moderate temperature difference between the solid and fluid phases highlights the excellent heat transfer performance of the open-cell architecture and supports the validity of the coupled electro-thermal modeling approach.

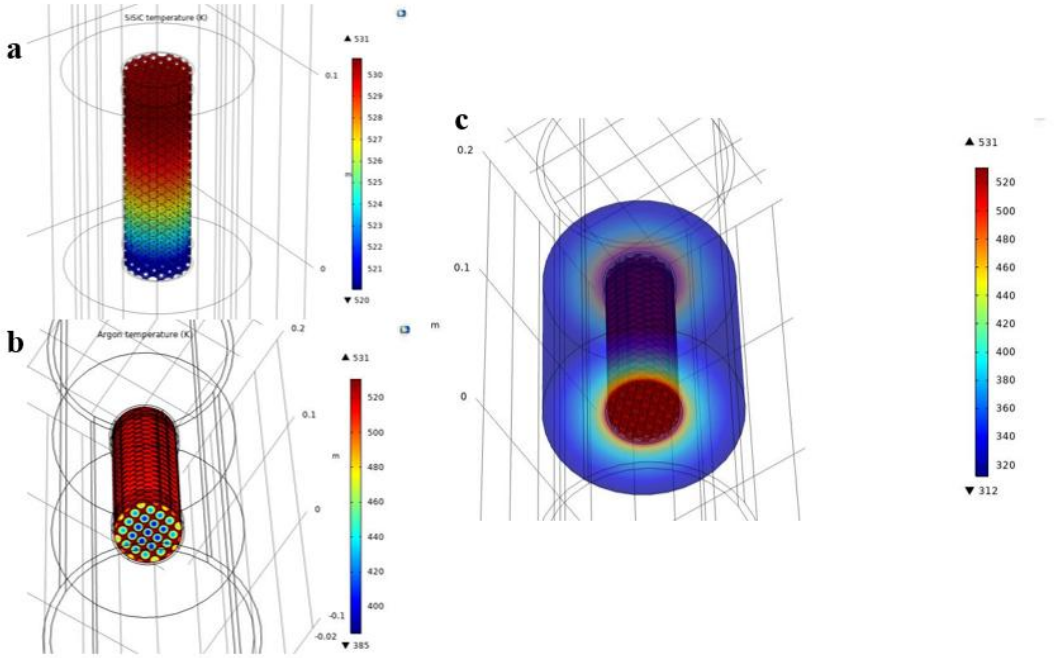


Figure 1. 3D spatial temperature distribution at steady state: (a) SiSiC structured matrix; (b) Argon gas phase; (c) complete reactor domain including the wall and external glass wool insulation.

4. Conclusions

This work demonstrates the feasibility of a multiphysics FEM approach in characterizing the electro-thermal response of SiSiC structured catalysts under Joule heating conditions. The model successfully captures the volumetric heat generation and the efficient solid-gas heat exchange, validated by the moderate temperature gradients observed. These results provide a robust foundation for optimizing electrified reactor geometries. Future developments will focus on investigating the influence of key geometrical parameters, such as porosity and cell density, on local electric field distribution, current pathways, and resulting temperature uniformity. In addition, the model will be extended to include catalytic reaction kinetics to assess the coupling between electro-thermal behavior and hydrogen production performance.

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ENHANCED PHOTOCATALYTIC HYDROGEN PRODUCTION FROM GLYCEROL OVER G-C_3N_4 PREPARED BY SUPERCRITICAL CO_2 MICRONIZATION ROUTE - (C172)

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Keywords: graphitic carbon nitride, photocatalysis, hydrogen production, glycerol photoreforming.

1. Introduction

Hydrogen represents a useful energy carrier for the sustainable transition due to its high energy density and the absence of direct CO_2 emissions during its use; heterogeneous photocatalysis constitutes a sustainable strategy for green H_2 production. The g-C_3N_4 photocatalyst is interesting for its stability and response to visible light, but its activity is limited by the recombination of electron-hole pairs. In the literature, this limitation has been addressed through coupling with co-catalysts or semiconductors, capable of promoting charge separation and increasing H_2 production. This work proposes the SAS micronization of urea with supercritical CO_2 as a precursor pretreatment to improve the performance of g-C_3N_4 in H_2 production from aqueous glycerol solutions, used as a sacrificial agent.

2. Materials and Methods

Untreated urea and urea treated by SAS with supercritical CO_2 were calcined to obtain g-C_3N_4 photocatalysts, subsequently characterized by SEM, FT-IR, UV-Vis DRS and XRD. Photocatalytic H_2 production was evaluated in a Pyrex batch reactor using 0.04 g of catalyst suspended in 40 mL of an aqueous solution containing 2 g of glycerol, N_2 as carrier gas, and irradiation by eight 8 W UV LED lamps emitting at 365 nm for 4 h and visibile. The data were collected using a gas analyzer connected to LabView software.

3. Results and Discussion

The SAS treatment produced different morphologies depending on the operating conditions, with 90 bar and 40 °C identified as the optimal condition for the experiments; well-defined and well-separated elongated structures were obtained, indicating a favourable balance between nucleation and growth. SAS-processed samples showed the best photocatalytic performance, being more active than the untreated sample. After 240 min of irradiation, H_2 production reached 8752 µmol L^{-1} for the SAS catalyst, compared with 3778 µmol L^{-1} for the non-SAS catalyst. This improvement can be attributed to a combination of morphological and optical factors.

The maximum catalytic efficiency was observed at 1 g L^{-1}, which was therefore identified as the optimal value among those investigated, 0.5 and 1.5 g L^{-1}. The comparison between UV and visible irradiation showed that the catalyst performed better under UV light. Photocatalytic tests were also carried out by varying the glycerol amount in order to identify, under the same operating conditions and catalyst dosage, the optimal concentration for hydrogen production. The maximum catalytic efficiency was observed at 5 wt% glycerol, which was therefore identified as the optimal value among those investigated, 2.5 wt% and 10 wt%.

To clarify the origin of the produced hydrogen, tests were carried out in deuterated water using the SAS catalyst at the optimal concentration of 1 g L^{-1} under UV irradiation. Replacing H_2O with D_2O caused a marked decrease in H_2 production, from 8752 µmol L^{-1} to 3259 µmol L^{-1} after 240 min, while CO_2 formation remained almost unchanged, decreasing only from 236 µmol L^{-1} in



H_2O to 232 µmol L^{-1} in D_2O. These results indicate that water is the main proton source for H_2 evolution, while glycerol mainly acts as a sacrificial agent and electron donor, contributing to charge separation and the formation of oxidized products.

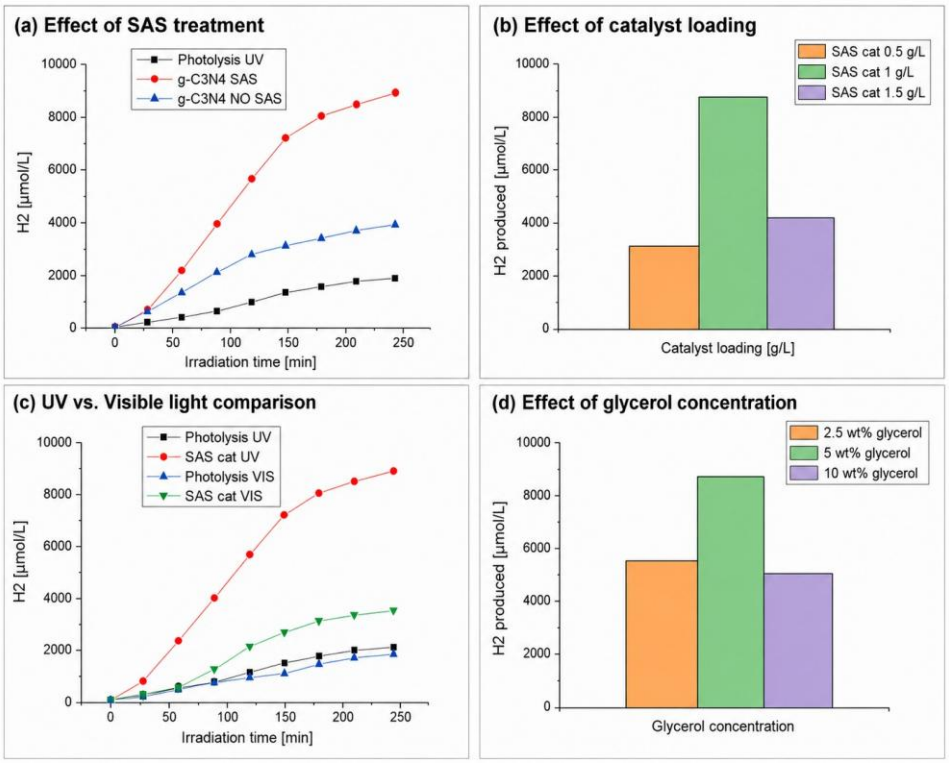


Figure 39: Photocatalytic H_2 production over g-C_3N_4 catalysts: effect of SAS treatment (a), catalyst loading (b), irradiation source (c) and glycerol concentration (d).

4. Conclusions

In conclusion, the SAS technique improves the photocatalytic activity of g-C_3N_4 for hydrogen production with glycerol. Using 1 g L^{-1} of SAS-processed g-C_3N_4, hydrogen production under UV irradiation doubled, reaching 8752 µmol L^{-1} in 240 min compared with the untreated material. Isotopic tests with deuterated water clarified that water mainly supplies the protons for H_2 generation, while glycerol acts as a sacrificial agent. Therefore, the SAS technique is confirmed as an effective pretreatment strategy to optimize g-C_3N_4 for sustainable hydrogen production.

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SUSTAINABLE BIO-MOF-DERIVED CARBON NANOFIBROUS ELECTROCATALYSTS FOR VANADIUM REDOX FLOW BATTERIES - (C173)

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Keywords: vanadium redox flow batteries, Bio-MOFs, carbon nanofibres, electrocatalysis, sustainable energy storage.

1. Introduction

Vanadium redox flow batteries (VRFBs) are attractive for large-scale stationary storage because of their long lifetime, rapid response and independent sizing of power and capacity. However, commercial carbon electrodes still suffer from sluggish V(II)/V(III) and VO^{2+}/VO_2^+ kinetics, which limits operation at high current density [1-3].. In order to avoid the use of cobalt- and nickel-based critical raw materials, the activity focused on CRM-free Bio-MOF precursors based on Zn-, Fe- and cyclodextrin/amino-acid frameworks. In particular, Zn–adeninate Bio-MOF-1, Zn–glutamate MOF and γ-cyclodextrin-derived MOF were selected as sustainable sacrificial templates for the preparation of heteroatom-doped porous carbon electrocatalysts. These systems are expected to provide N/O/S-rich surface functionalities, improved wettability, hierarchical porosity and enhanced charge-transfer kinetics toward vanadium redox reactions, while avoiding CRM-containing catalytic nodes

2. Materials and Methods

Bio-MOF precursors were prepared from biomolecular ligands and non-noble metal salts, dispersed in PAN-based spinning solutions and processed by electrospinning. The fibrous mats were stabilized and pyrolysed to obtain heteroatom-doped carbon nanofibres. Structure and morphology were investigated by XRD, SEM, TEM, XPS, TGA and BET, while electrochemical behaviour was assessed by cyclic voltammetry, EIS and VRFB single-cell cycling.

3. Results and Discussion

The activity delivered continuous carbon nanofibrous electrodes decorated with MOF-derived catalytic domains. SEM/TEM analyses showed interconnected fibres with diameters of 180-320 nm, while BET measurements indicated a surface area of 315 $m^2 g^{-1}$. XPS confirmed the presence of N- and O-containing functional groups (4.8 and 9.6 at%, respectively), which are expected to promote vanadium redox kinetics. In single-cell VRFB tests, stable cycling was achieved from 50 to 200 mA cm^{-2}. At 150 mA cm^{-2}, the cell delivered CE = 98.3%, VE = 83.5% and EE = 82.1%. After 100 cycles at 150 mA cm^{-2}, the capacity retention was 88%, with no relevant increase in polarization. The main performance indicators are summarized in Table .

Table 1. Representative electrochemical results obtained with Bio-MOF-derived carbon nanofibrous VRFB electrodes.

Parameter	Pristine GF	Bio-MOF-CNF electrode	Project target
Fibre diameter	-	180-320 nm	continuous fibrous network
BET surface area	18 $m^2 g^{-1}$	315 $m^2 g^{-1}$	high active area
EE at 150 mA cm^{-2}	74.6%	82.1%	>80%
CE at 150 mA cm^{-2}	96.7%	98.3%	90-100%
Capacity retention	79% after 100 cycles	88% after 100 cycles	>70% DoD/SoD



4. Conclusions

The results demonstrate that Bio-MOF-derived carbon nanofibres can combine sustainable precursor selection, scalable electrospinning and enhanced electrocatalytic activity for VRFBs. The reduced Rct, improved reversibility and EE above 80% at 150 mA cm^{-2} highlight their potential as low-cost electrode modifiers for high-efficiency stationary energy-storage systems.

Acknowledgements

This work was supported by the Italian Ministry for the Environment and Energy Security (MASE) and CNR within the "Accordo di Programma MASE–CNR per la Ricerca del Sistema Elettrico Nazionale" (PTR 2025–2027).

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HARMONIZED TEST PROTOCOLS AND TRAINING PROGRAMS FOR GREEN HYDROGEN PRODUCTION, STORAGE/CONVERSION AND FUEL CELL TECHNOLOGIES - (C177)

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Keywords: harmonized test protocols, green hydrogen value chain, electrolysis and photo(electro)catalysis, hydrogen storage and carriers, fuel cells, technical and scientific training.

1. Introduction

The transition toward a mature hydrogen economy depends not only on continuous progress in functional materials and devices, but also on robust, mutually comparable and reproducible test methodologies able to bridge ex-situ material screening with component-, prototype- and system-level validation, together with a technically skilled workforce able to sustain the sector's growth. Within the PORH2 project, CNR coordinated a multi-institute activity that defined harmonized test protocols across the entire green-hydrogen value chain – production, storage/conversion and utilization in fuel cells – paired with structured training pathways for technical-diploma holders, graduates, PhD students and private-sector personnel.

2. Materials and Methods

For green H_2 production (electrolysis, biological, gasification/reforming, photoelectrochemical and photocatalytic processes), ex-situ protocols addressed the chemical, physical, morphological, structural and surface properties of catalysts, electrocatalysts, semiconductors, electrolytes and biomass feedstocks, complemented by cyclic voltammetry, polarization curves, electrochemical impedance spectroscopy (EIS) and accelerated ageing tests; subsequent protocols targeted electrode–electrolyte assemblies, catalytic beds and semiconductor–electrolyte interfaces, followed by prototype-level testing of catalytic/biological reactors, photo(electro)catalytic devices and electrolysis stacks, and finally by full-system validation.

For H_2 storage and conversion (power-to-gas, catalytic/photocatalytic conversion into liquid organic and nitrogen-based carriers, biological processes, solid-state storage in metal hydrides/MOFs), analogous protocols were extended to electronic properties and storage efficiency, with multi-scale (micro- and bench-scale) catalytic test rigs used to correlate catalytic performance with the porosity, layer thickness and loading of structured catalysts, up to reactor/stack- and system-level validation.

For fuel cell utilization (low- and high-temperature), protocols covered specific resistance and conductivity for electrolytes, electrocatalytic parameters (active surface area, Tafel slope, exchange current density, charge-transfer resistance) for catalysts, electrode–electrolyte assembly polarization and durability, and stack-level diagnostics via complex impedance spectroscopy, including bipolar-plate stability, up to system-level validation.

In parallel, three training lines built a shared, three-tier professional pipeline (technical-diploma holders; graduates and PhD students, including dedicated industrial PhD positions and research grants; private-sector personnel), combining a common foundational module (chemistry, electrochemistry, physics, chemical reactors, transport phenomena, R&D project management) with hands-on involvement in characterization, prototyping and monitoring activities and participation in international conferences.

3. Results and Discussion



Across the three technology pillars, the framework progressively delivered validated protocols and performance indicators – first at material level (months 3–15), then at component level (months 21–24), prototype level (months 30–36) and finally system level (months 39–42) – raising the overall Technology Readiness Level (TRL) from 2 to 4 across all three pillars. In parallel, the training lines recruited at least 4 industrial-PhD/research-grant contracts per pillar (12 overall) and delivered dedicated courses for diploma holders, graduates/PhD students and private-sector personnel, culminating in at least 4 newly trained experts per pillar (12 overall) skilled in the design and development of innovative green-hydrogen methods and techniques.

Scope	Materials, components, prototypes and complete systems
Processes	Electrolysis, electroreforming, catalytic gasification/reforming, biological, PEC and photocatalytic routes
Material screening	Ex situ characterization; catalytic, photocatalytic, biological and electrochemical activity tests
Electrochemical diagnostics	CV, polarization curves, EIS, crossover, stability and accelerated stress tests
Prototype validation	Performance, durability and dynamic behaviour; in situ spectroscopy
Synthetic indicators	Efficiency, stability, degradation and dynamic response descriptors

Table 1. Main elements of the harmonized protocol framework for green hydrogen production technologies.

4. Conclusions

A coordinated, harmonized test-protocol framework spanning green-hydrogen production, storage/conversion and fuel cell utilization, integrated with a three-tier training pathway, was implemented and provided standardized TRL 2–4 methodologies together with a critical mass of trained experts. This approach enabled reliable, mutually comparable benchmarking of materials, components, prototypes and systems developed by different research groups, supporting the scale-up of green-hydrogen technologies and the growth of a qualified workforce for the hydrogen economy.

Acknowledgements

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IONIC LIQUID-MODIFIED HYBRID POLYMERIC MATERIALS FOR THERMAL ENERGY STORAGE APPLICATIONS - (C181)

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Keywords: Ionic liquids, Hybrid polymeric materials,Thermal energy storage.

1. Introduction

The growing demand for sustainable energy technologies has stimulated the development of advanced materials for thermal energy storage (TES). Among the most promising solutions, hybrid materials combining polymeric matrices and phase change materials (PCMs) offer the possibility of storing and releasing large amounts of thermal energy while maintaining structural stability. However, the performance of these systems is often limited by poor thermal conductivity, phase segregation, and mass-transfer resistance. In this context, ionic liquids (ILs) have emerged as attractive functional additives due to their negligible vapor pressure, high thermal stability, tunable physicochemical properties, and affinity toward water and other polar compounds.

This work investigates the incorporation of ionic liquids into electrospun polymeric structures designed as supports for advanced PCM-based hybrid materials. The objective is to evaluate the role of ILs as multifunctional additives capable of enhancing thermal storage performance, moisture sorption behavior, and overall material stability.

2. Materials and Methods

Hybrid polymeric materials were prepared by electrospinning polyacrylonitrile (PAN)-based solutions containing different concentrations of the ionic liquid 1-Ethyl-3-methylimidazolium acetate ([EMIM][Ac]). The polymer solutions were prepared in dimethylformamide (DMF) and processed under optimized electrospinning conditions to obtain homogeneous fibrous mats.

The resulting materials were characterized in terms of morphology, structural integrity, and water adsorption/desorption performance. Scanning Electron Microscopy (SEM) was used to investigate fiber morphology, while sorption measurements were performed under controlled humidity and pressure conditions. The developed fibrous structures are intended to serve as functional matrices for the subsequent incorporation of phase change materials in advanced TES systems.

3. Results and Discussion

The addition of ionic liquid influenced both the morphology and functional properties of the electrospun fibers. SEM analyses revealed that increasing IL concentration led to larger fiber diameters and a gradual modification of fiber organization, while maintaining the integrity of the fibrous network. The ionic liquid was successfully retained within the polymeric structure, indicating good compatibility between the two components.

Water adsorption tests showed a significant increase in moisture uptake with increasing IL content, demonstrating the active contribution of the ionic liquid to mass-transfer processes. These findings suggest that ILs can effectively act as multifunctional additives, improving the physicochemical characteristics of polymeric supports intended for thermal energy storage applications.

The incorporation of ionic liquids into electrospun polymeric matrices represents a promising strategy for the development of advanced hybrid materials for energy applications. The results demonstrate that ILs can enhance sorption properties while maintaining structural stability, making them suitable functional additives for PCM-containing systems. Future work will focus on the integration of multiple PCMs within the polymeric matrices and on the optimization of polymer–PCM–ionic liquid interactions to maximize thermal storage capacity and long-term operational performance.

Acknowledgements

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AN INTEGRATED EXPERIMENTAL AND MOLECULAR DYNAMICS APPROACH TO CORRELATE OXIDE-ION FRAMEWORK AND FUNCTIONAL PROPERTIES IN DOPED SRFEO3 ELECTROCATALYSTS - (C188)

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Keywords: Perovskite oxide, ionic conductivity, SOFC.

1. Introduction

Solid oxide fuel cells (SOFCs) offer a viable route to sustainable energy production thanks to their high electrical efficiency and broad fuel flexibility. To render SOFCs competitive, improving the oxygen reduction reaction (ORR) of electrocatalysts remains essential. Optimizing the oxide perovskite composition, the most promising class of electrocatalysts, enables targeted tuning of structural, electronic, and defect-related properties that control catalytic activity and mixed ion–electron conduction. This work concerns the study of Al-doped $SrFeO_3$ combining experimental studies and molecular dynamics simulations at operating temperature with the aim of correlating starting material properties - oxide ions localization and environment - ionic conduction processes at high temperatures.

2. Materials and Methods

$SrFe_{0.9}Al_{0.1}O_3$ and $Sr_{0.9}Sm_{0.1}Fe_{0.9}Al_{0.1}O_3$ were synthesized by solution combustion synthesis. Structural, textural and reduction properties were investigated by X-ray diffraction with Rietveld analysis, thermogravimetric analysis and H_2-temperature programmed reduction. Electrochemical impedance spectroscopy tests were carried out in air. Classical molecular dynamics simulations were performed on isothermal–isobaric ensemble at 1200 K by using Buckingham potential coupled Coulombic interactions.

3. Results and Discussion

X-ray diffraction associated with Rietveld analysis evidences the incorporation of dopants in the cubic perovskite crystal structures for both studied compositions. Even though Al^{+3} has a smaller ionic radius (0.535Å CN=6) lower than Fe^{+4} (0.585 Å, CN= 6), its incorporation causes an increase in the unit-cell volume. Further introduction of Sm^{3+} (1.24 Å, CN = 12) leads to an additional expansion of the lattice parameters. The lattice expansion is likely driven by charge compensation through partial reduction of Fe^{4+} to Fe^{3+} (0.645 Å, CN = 6) and by the concomitant formation of oxygen vacancies, which increase the average cationic radius and produce lattice dilation. Oxygen vacancies formation is beneficial for ORR and for oxygen ions transport. It is possible to assess the suprafacial and partially bulky oxygen vacancies amount by TGA analysis; experimental data indicate slightly higher oxygen-vacancies content for $SrFe_{0.9}Al_{0.1}O_3$ with respect to $Sr_{0.9}Sm_{0.1}Fe_{0.9}Al_{0.1}O_3$. This behavior likely arises from aliovalent Al^{3+} and Sm^{3+} substitution, which promotes oxygen-vacancy formation and Fe^{4+}/Fe^{3+} reduction, respectively. Considering that iron is the only reducible species, $Sr_{0.9}Sm_{0.1}Fe_{0.9}Al_{0.1}O_3$ exhibits a higher reducibility by H_2-TPR than $SrFe_{0.9}Al_{0.1}O_3$, as evidenced by hydrogen consumption at 450°C. Moreover, the observed shift of reduction peak toward low temperatures indicates enhanced oxygen mobility for $Sr_{0.9}Sm_{0.1}Fe_{0.9}Al_{0.1}O_3$ with respect to $SrFe_{0.9}Al_{0.1}O_3$. Accordingly, electrochemical impedance spectroscopy tests in air between 700-850°C evidence lower resistances for $Sr_{0.9}Sm_{0.1}Fe_{0.9}Al_{0.1}O_3$ with respect to $SrFe_{0.9}Al_{0.1}O_3$ hinting at a higher ion mobility in



Sm-doped sample. Electrochemical impedance spectroscopy studies conducted on $SrFe_{0.9}Al_{0.1}O_3$ are consistent with the ion diffusion data obtained via molecular dynamics simulations, and oxygen-vacancy clustering around Al may reduce oxygen-ion mobility increasing resistance.

4. Conclusions

In conclusion, the case study on $SrFe0_{.9}Al_{0.1}O_3$ and $Sr_{0.9}Sm_{0.1}Fe_{0.9}Al_{0.1}O_3$ for the oxygen reduction reaction (ORR) provides an opportunity to correlate structural, reducibility, and electrochemical impedance spectroscopy properties with the localization and environment of the oxide ions, as determined by molecular dynamics simulations. $Sr_{0.9}Sm_{0.1}Fe_{0.9}Al_{0.1}O_3$ appears to be the most promising candidate, making it the most interesting composition for further investigation.

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GREEN HYDROGEN GENERATION AND BIOMASS DEGRADATION VIA A PHOSPHOMOLYBDIC ACID-MEDIATED ELECTROCHEMICAL APPROACH - (C189)

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Keywords: hydrogen, electrolysis, biomass.

1. Introduction

Biomass-assisted water electrolysis (BAE) is increasingly competitive with traditional green hydrogen, costing $2.50–$3.50/kg for H_2 [1]. This economic viability stems from a diversity of available, renewable feedstocks. Abundant lignocellulosic biomass remains the most promising, scalable source despite needing pre-treatment. BAE achieves these economic advantages by replacing standard anodic oxygen evolution with the oxidation of organic substrates. This fundamental shift slashes required cell voltages from over 1.8 V to roughly 0.6–0.7 V. Consequently, it reduces the energy consumption of conventional electrolysis (4.8 kWh/Nm^3 H_2) by up to three times, representing a sustainable evolution in water-splitting technology.

2. Materials and Methods

The investigation evaluated diverse lignocellulosic substrates—including steam-exploded lignin, commercial cellulose, hemicellulose, paper mill sludge, and pulverized hazelnut shells—to demonstrate the electrochemical versatility across varying biomass structures. Each feedstock underwent an aqueous oxidative pretreatment at 100 °C using phosphomolybdic acid (PMA) as a redox mediator. During this phase, the biomass oxidized, transferring its stored electrons to chemically reduce the PMA. Subsequently, the process transitioned to an H-type electrolysis cell. At an ambient 25 °C and a low cell potential of 0.7 V versus SHE, the reduced PMA was re-oxidized at the anode, while pure hydrogen evolved at the cathode. Crucially, the PMA acts as a true, unconsumed mediator that fully regenerates for continuous reuse. Structural degradation of the biomass into simpler organic fragments was verified using GC-MS and HPLC. Reaction yields and hydrogen volumes were quantified through bulk electrolysis, chronoamperometry, and Linear Sweep Voltammetry (LSV). Finally, calculated specific oxidation efficiencies was calculated and experimental charge exchange data was compared against a theoretical baseline of available electrons, which was established via elemental analysis of the raw materials.

3. Results and Discussion

In this work, we propose a mediated electrochemical approach using phosphomolybdic acid (PMA) to valorize lignocellulosic biomass and biorefining byproducts [2]. This method couples low-voltage hydrogen generation with complex organic matter degradation, transforming raw feedstocks into value-added chemicals while maintaining high energy efficiency. By maintaining a constant potential, we calculated the electrical energy consumption at 67 MJ/kg H_2. This requirement is markedly lower than the demand of conventional water electrolysis systems, which operate at significantly higher potentials. This reduction in energy expenditure suggests the PMA-mediated approach provides a more economically competitive and environmentally sustainable pathway for producing green hydrogen from renewable waste.



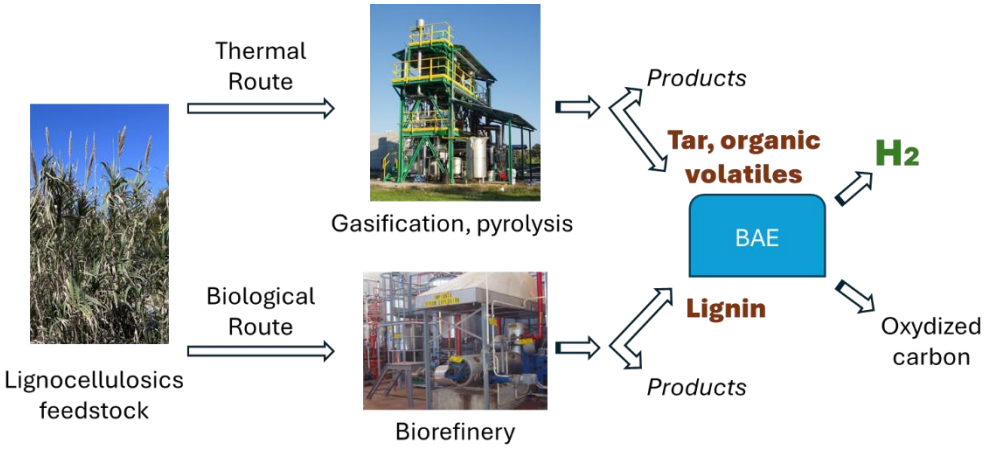


Figure 1: Production of hydrogens by BAE from byproduct of lignocellulose conversion. In the upper the updraft gasification plant PRAGA, at the lower the steam explosion digester, both pilot facilities at ENEA CR of Trisaia.

4. Conclusions

By successfully coupling distinct chemical processes, this system overcomes many thermodynamic hurdles affecting conventional hydrogen production. These comprehensive findings underscore that applying PMA as a catalytic mediator for the oxidative degradation of complex lignocellulosic structural matrices is an advantageous strategy. Ultimately, this methodology proves uniquely effective by integrating the high-value transformation of organic waste with the energy-efficient generation of hydrogen gas at remarkably low electrochemical potentials.

Acknowledgements

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CATALYTIC SUPERCRITICAL WATER GASIFICATION OF WET AGRO-INDUSTRIAL RESIDUES: TAILORING RENEWABLE GAS PRODUCTION THROUGH Ni-BASED CATALYSTS - (C195)

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Keywords: Ni-based catalysts, 3D structured catalysts, gasification under supercritical water

1. Introduction

The sustainable valorization of wet agro-industrial residues is attracting increasing attention as an alternative to conventional waste disposal owing to their high moisture content and significant organic fraction. Unlike conventional thermochemical technologies, Supercritical Catalytic Water Gasification (SCWG) enables the direct conversion of wet biomass without energy-intensive drying, taking advantage from the action of water simultaneously as solvent, reactant and hydrogen donor above supercritical point ($T > 374$ °C, $P > 22.1$ MPa). In this work, an integrated biorefinery strategy is proposed by coupling a green extraction step for the recovery of high-value compounds from biomass residues with SCWG for the conversion of the remaining organic fraction into renewable gaseous fuels. Particular attention is devoted to the development of Ni-based catalysts and structured catalytic architectures capable of tuning product selectivity and improving process operability.

2. Materials and Methods

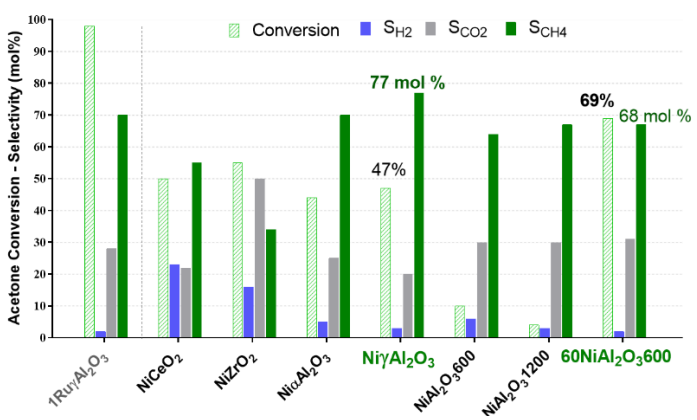
Citrus processing residues (pastazzo) were selected as representative wet agro-industrial biomass. Green extraction was performed using ethanol/water mixtures and ultrasound-assisted extraction to recover valuable compounds such as D-limonene and polyphenols while preserving most of the organic matter for subsequent energy conversion. The residual organic fraction was investigated under SCWG conditions using acetone as a model oxygenated compound. Catalytic tests were carried out at 450 °C and 30 MPa employing Ni-based catalysts supported on γ-Al_2O_3, CeO_2 or ZrO_2 being prepared by impregnation or coprecipitation methods. Product distribution (H_2, CH_4 and CO_2) was evaluated as a function of catalyst composition and preparation route. To improve catalyst handling under supercritical conditions, structured catalysts were fabricated by robocasting and fully characterized from an analytical, morphological and structural point of view.

3. Results and Discussion

The extraction step successfully recovered valuable bio-based compounds from about 7% of the total organic matter, leaving approximately 93% of the organic fraction available for subsequent gasification. Ultrasound-assisted extraction enhanced D-limonene recovery, whereas EtOH-H_2O mixtures efficiently extracted polyphenols without significantly affecting the energy potential of the residual biomass. Catalytic SCWG experiments demonstrated that catalyst formulation strongly influences the reaction pathways. Ni catalysts supported on Al_2O_3 mainly promoted methanation, reaching CH_4 selectivities up to 70–77 mol%, whereas CeO_2 and ZrO_2 favored reforming and water-gas shift reactions, shifting the product distribution toward H_2 with selectivities up to 20–30 mol%. The catalyst preparation method also affected catalytic performance. Coprecipitated catalysts exhibited stronger metal-support interactions, enhanced reducibility and improved activity compared with impregnated materials. As for the potential of Ni-based structured monoliths, SEM-FIB observations and EDX mapping confirmed a homogeneous distribution of the active phase throughout the printed structures while preserving geometry and mechanical integrity. Catalyst structuring initially caused a decrease in activity because of the lower amount of active phase available on the surface. However, this limitation was overcome by increasing the catalyst loading. With two structured monoliths, acetone conversion increased up to



91%, while maintaining a high methane selectivity of around 67 mol%. These structured catalysts represent promising candidates for continuous SCWG reactors by improving catalyst handling and reducing plugging issues.



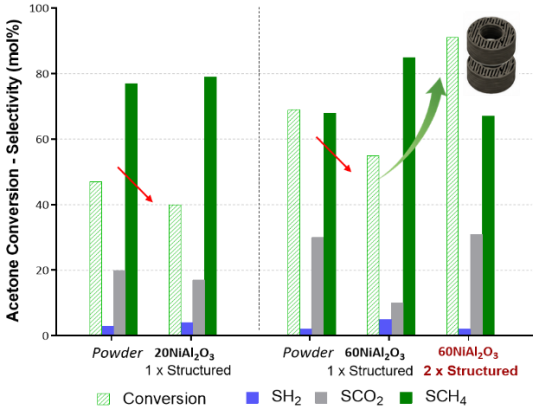


Figure 1. Comparison of powdered catalysts [left] and structured catalysts [right] in the SCWG of acetone at 425 °C. Reaction conditions: V_R = 75 mL, organic phase loading =10 vol/vol, $R_{cat/org}$ = 0.6 g g^{-1}, time = 20 min.

4. Conclusions

An integrated approach combining green extraction and catalytic supercritical water gasification has been successfully developed for the sustainable valorization of wet agro-industrial residues. The preliminary extraction step efficiently recovers valuable bio-based chemicals while preserving most of the organic carbon for energy conversion. Subsequently, Ni-based catalysts resulted to be able in the conversion of residual fraction into renewable gaseous fuels, with catalyst composition governing the balance between methane production and hydrogen generation. Moreover, the successful fabrication of structured catalysts offers a promising strategy for improving catalyst stability, process operability and future scale-up of SCWG technology.

Overall, the results demonstrate that both catalyst composition and architecture provide effective tools for tailoring the H_2/CH_4 ratio according to the desired energy application.

Acknowledgements

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REPUCOMP: COMBINED POLYURETHANE RECYCLING AND SEWAGE SLUDGE VALORIZATION THROUGH THERMOCHEMICAL VALORIZATION – (C205)

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Keywords: polyurethane recycling, pyrolysis, syngas, biochar.

1. Introduction

Polyurethane (PU) synthesis is widely used to manufacture insulation panels, construction foams, and insulated household appliances. Production of PU-based goods, with flexible and rigid foams at European Union generates around 675 ktons of PU waste annually, two-thirds of which still ends up in landfills due to recycling challenges. At the same time, global demand for polyols, a key PU feedstock, has reached 11 Mtons per year. Conventional fossil-based polyol production relies heavily on petroleum resources and generates significant CO_2 emissions, driving interest in bio-based and recycled polyols. However, many biopolyols are still derived from virgin vegetable oils, prompting industry to seek more sustainable alternatives that reduce environmental impacts and supply chain emissions.

RePUComp project aims to develop technology for the efficient chemical recycling of polyurethane-containing composites. Several waste streams have been identified and explored for conversion efficiency and novel downstream applications of the recovered chemicals. The aim is to integrate green solvothermal liquefaction and downstream pyrolysis technologies to enable the efficient recycling of select mixed waste streams towards new applications within industrial polyurethane, such as flexible and rigid foams - promoting sustainability and innovation within the sector. In this contribution, we focus on the development and validation of a pyrolysis process for coprocessing the solid waste from biopolyol synthesis[1] and the solid waste generated from PU glycolysis. The biochar obtained from this process will be used as basic catalyst for the glycolysis process, ensuring circularity, while the pyrolysis liquids will be evaluated as potential source of biopolyols, reducing environmental impact via by-product utilization. Heat duty of the process is to be met by burning the syngas generated during pyrolysis. The validation of this valorization scheme has been recently demonstrated for the solid waste of biopolyol[2], and this knowledge will be herein transferred for the valorization of the waste of the PU glycolysis process.

2. Materials and Methods

A schematic diagram of the pyrolysis unit designed and constructed for this project is shown in Figure 1. The system consists of a vertical furnace with three independently heated zones, providing an isothermal region of at least 80 cm within the reactor. The feedstock is placed in a sample holder located at the center of an Inconel 600 tube, measuring 100 cm in length and 2.3 cm in inner diameter. For the initial studies, 25 grams of the solid filter cake obtained from the production of biopolyols via the acid liquefaction of sugar beet pulp was used. The recovery procedure for this material has been described elsewhere[1]. A mass flow controller supplies an inert gas, allowing the residence time of the pyrolysis vapors within the furnace's hot zone to be adjusted. At the reactor outlet, a train of six condensers connected in series—one cooled with isopropanol (IPA) and five water-cooled, with the last two maintained at 0 °C—collects the condensable products generated during pyrolysis. The non-condensable gases subsequently pass through a cotton filter, and the concentrations of CO, CO_2, CH_4, and H_2 are continuously monitored. The presence of C_2–C_4 hydrocarbons, H_2S, acetaldehyde, and nitrogen-containing gases is determined by GC–FID–MS analysis using gas samples collected in Tedlar bags.



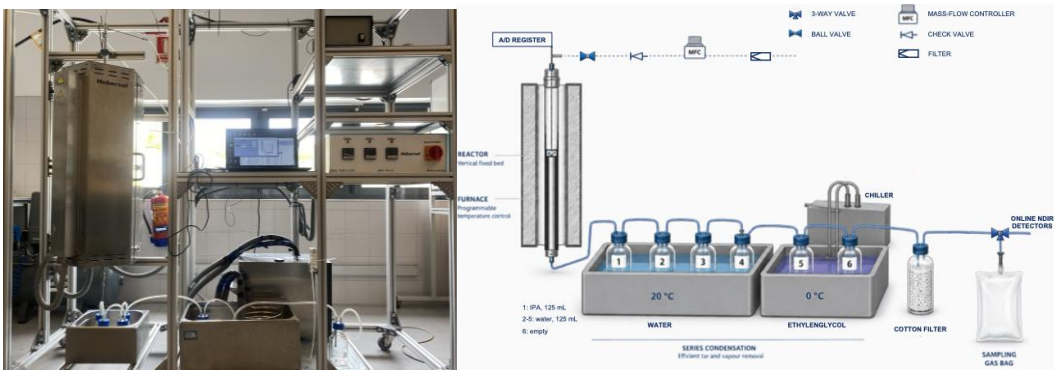


Figure 1. Pyrolysis system built for RePUComp project.

3. Results and Discussion

The first experimental campaign has been successfully completed, delivering solid yield of 22-25%, liquid yield of 60-65%, and gas yield of 10-15%. The resulting biochar shows a high concentration of alkali and alkaline earth metals, totaling 37 %wt, and surface area of ca. 25 m^2/g. The liquid stream is fractionated into water-soluble and water-insoluble compounds, being more than 80% soluble in water. The oxygenated hydrocarbons stream have a low hydroxyl number, which could be improved by further fractionation. The gas stream has a lower LHV than expected, rendering necessary to burn around 20% of the liquid fraction to meet the heat duty of the process.

4. Conclusions

A slow pyrolysis process for filtered residues of bipolyol and glycolysis processes has been successfully deployed, enabling the characterization of all the pyrolysis fractions.

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