

# ESEE 2021

12<sup>TH</sup> EUROPEAN SYMPOSIUM ON ELECTROCHEMICAL ENGINEERING  
Electrochemistry for electrification and energy transition towards a sustainable future

## Program & abstracts

June 14-17, 2021

organized by



in cooperation with



in partnership with



sponsored by



Leeuwarden, June 2021

Dear colleagues,

It is our pleasure to welcome you this week to ESEE 2021, the 12th European Symposium on Electrochemical Engineering, to be held 14-17 June, 2021, online in Leeuwarden, The Netherlands. We are pleased to present to you the book of abstracts of the conference, containing detailed descriptions of the presentations of this week.

It has been two years of preparation, but now ESEE 2021 has finally arrived!

In April 2020, we were ready to host a vibrating conference in Leeuwarden, the charming capital city of Friesland in the north of The Netherlands. We would have loved to welcome you at Wetsus, and share with you our research and vision for electrochemical engineering, for industrial and environmental applications.

But it was not to be that way. Instead, over the past months, we have decided to transform ESEE to a fully online event. Luckily, the quality of the scientific program has not changed at all, and we are proud today to present a 4-day live online event with more than 130 speakers, 70 posters, 8 plenary talks, and 15 keynotes, with presenting authors not only from Europe, but from all continents.

We hope that you will enjoy the conference and – although online – you will all feel part of the electrochemical engineering community and this conference, not as observers, but as real participants.

Please during the upcoming week, take your time to interact with other participants, visit the exhibition hall, and join the poster and matchmaking sessions.

We look forward to meeting you online this week, and discuss our scientific research.

Finally, we wish you an enjoyable time participating in ESEE 2021!

On behalf of the ESEE 2021 organizing committee,

Yours sincerely,

*Michele Tedesco (chair)*

*Maarten Biesheuvel (co-chair)*

*Bert Hamelers (co-chair)*



## Day 1: Monday 14 June

Click on the title to go to the abstract

09:00 - 09:20	<b>Opening</b>		
09:20 - 10:00	<b>Plenary: W. Nitschke, Life's emergence: an early success story of electrochemical free energy conversion</b>		
10:00 - 11:00	<b>Session 1: Advances in vanadium redox flow batteries</b> <i>Chair: A. Forner-Cuenca</i>	<b>Session 2: Electrochemical degradation and disinfection processes</b> <i>Chair: M. Rodrigo</i>	<b>Session 3: Water electrolysis and fuel cells - I</b> <i>Chair: W. Haverkort</i>
10:00 - 10:15	555 M. Bureš, Mitigation of capacity and efficiency loss in vanadium redox flow batteries: mathematical model and experimental validation	516 N. Duinslaeger, Graphene Sponge Electrodes for Electrochemical Degradation of Perfluoroalkyl Substances (PFAS)	164 D. Franzen, Spatially resolved model for oxygen reduction reaction in porous gas-diffusion electrodes
10:15 - 10:30	340 C. Weidlich, Half-Cell Monitoring at All-Vanadium-Flow-Batteries (VFB)	430 G. Norra, Electrochemical Disinfection of E. Coli with Reduced Graphene Oxide Foam Electrodes	204 F. Kubannek, Effect of Carbon Dioxide from Ambient Air on Alkaline Exchange Membranes for Fuel Cells
10:30 - 10:45	231 E. Prumbohm, Optimisation of flow field designs for vanadium redox-flow batteries	248 M. Herraiz Carbone, Photo-assisted electrochemical disinfection of hospital urines using a novel flow-through reactor	114 C. Sánchez Martínez, Overcoming mass transport limitations in electrochemical reactors with a pulsating flow electrolyzer
10:45 - 11:00	206 I. Kroner, Investigations on the vanadium ion reaction kinetics on single carbon fibre electrodes	162 M. Mohseni, Fe <sub>3</sub> O <sub>4</sub> -incorporated carbon microtubes as efficient electrodes for the degradation of persistent pollutants at neutral pH	
11:00 - 11:20	<b>Coffee break</b>		
11:20 - 12:45	<b>Session 4: Advances in Li-ion and other batteries</b> <i>Chair: Y. Bultel</i>	<b>Session 5: Capacitive deionization: applications</b> <i>Chair: M. Biesheuvel</i>	<b>Session 6: Alkaline water electrolysis</b> <i>Chair: T. de Groot</i>
11:20 - 11:45	372 P. Thivel, Impact of batteries ageing on their state of security	618 M. Suss, Co-generation of electricity and desalted water using chemical energy	51 J. Haverkort, Rethinking Alkaline Water Electrolysers
11:45 - 12:00	563 H. Steinrück, Concentration and Velocity Profiles in a Polymeric Lithium-ion Battery Electrolyte	570 Y. Jande, Energy consumption for fluoride removal using constant current operated capacitive deionization system	607 J. Bleeker, Controlling gas bubble nucleation and release in alkaline electrolysis
12:00 - 12:15	524 N. Rigos, Effect of fast charging on Lithium plating and SEI growth	548 A. Shocron, Electrochemical removal of amphoteric ions	445 T. Rauscher, Highly active electrodes for alkaline water electrolysis by femtosecond-laser processing
12:15 - 12:30	449 P. Thivel, From first to second life of lithium-ion batteries study	527 Z. Sahray, Theory of monovalent ion selectivity using porous carbon capacitive deionization electrodes	326 A. Rajora, An analytical model for liquid and gas diffusion layers in electrolyzers and fuel cells
12:30 - 12:45			42 J. Brauns, Enhancing the part-load range of alkaline water electrolyzers by model-based optimization
12:45 - 14:00	<b>Lunch</b>		

14:00 - 14:40	<b>Plenary: M. Wessling, Electrochemical ammonia synthesis</b>		
14:40 - 15:40	<b>Session 7: Redox flow batteries</b> <i>Chair: D. Vermaas</i>	<b>Session 8: Electrochemical wastewater treatment</b> <i>Chair: S. Ucar</i>	<b>Session 9: Water electrolysis and fuel cells - II</b> <i>Chair: W. Haverkort</i>
14:40 - 14:55	558 P. Mazúr, Development of aqueous redox flow batteries based on organic electroactive compounds	595 J. Ma, Novel porous TiOx anode materials for the removal of organic pollutants from water	263 L. de Haart, Sustainable Syngas Production in Power-to-X Technologies
14:55 - 15:10	380 I. Leon-Sotelo, Simulation of hydrodynamics, mass transport and current distribution in a Cerium-Vanadium redox flow battery	502 Z. Gu, A biomimetic photocatalytic system for efficient electricity generation from wastewater treatment	256 S. Díaz Abad, Addressing the challenges of the SO <sub>2</sub> depolarized electrolysis at high temperature
15:10 - 15:25	255 J. Hereijgers, Improving the hydrodynamics of redox flow batteries through 3D printed electrodes	362 E. Lacasa, Development of electrochemical processes to reduce environmental risk of Hospital Effluents	226 L. Castañeda, Theoretical and experimental characterization of H <sub>2</sub> O-H <sub>2</sub> flow in an electrocoagulation reactor in serpentine array
15:25 - 15:40	150 J. Charvát, Effect of operating conditions on performance and lifetime of vanadium-oxygen fuel cell	260 J. Graves, Electrochemical oxidation of ammonia coupled with hydrogen generation	
15:40 - 16:00	<b>Coffee break</b>		
16:00 - 17:30	<b>Poster session</b>		

## Day 2: Tuesday 15 June

09:20 - 10:00	<b>Plenary: M. Zheludkevich, Complexants as active modulators of metal surface reactivity: from Corrosion Control to Primary Batteries</b>		
10:00 - 11:00	<b>Session 10: Advances in CO<sub>2</sub> electroreduction - I</b> <i>Chair: B. Mei</i>	<b>Session 11: Flow batteries and novel energy storage systems</b> <i>Chair: A. Forner-Cuenca</i>	<b>Session 12: Water electrolysis and fuel cells: materials</b> <i>Chair: C. Weidlich</i>
10:00 - 10:15	601 N. Ligthart, Suspension electrodes for enhanced mass transfer in electrocatalytic CO <sub>2</sub> reduction	605 A. Culcasi, Optimization study of acid-base flow battery stacks with monopolar and bipolar membranes	610 Z. Qiu, Promising Hydrogen Production from Black Liquor Electrolysis on Earth-Abundant Catalysts
10:15 - 10:30	537 M. Miola, Scalable Bismuth electrocatalyst for selective CO <sub>2</sub> -to-formate conversion	533 J. Steen, Stable Organic Radicals for Symmetric Redox Flow Batteries	196 M. Vagin, Proton and oxygen management in electrocatalysis on conducting polymers
10:30 - 10:45	330 M. Pupo, Role of Different Electrolytes in CO <sub>2</sub> RR – Improvements in FE and Product Selectivity	448 L. Gurreri, Lab-scale experiments on a novel acid/base electro-dialytic flow battery with bipolar membranes	93 M. Durovic, NiCoP cathode catalyst for electrochemical water splitting: Structural and electrochemical characterization
10:45 - 11:00	79 I. Katsounaros, Real-time characterization of CO <sub>2</sub> reduction products		71 F. Sapountzi, Metal phosphides as cathodes in PEM water electrolysis
11:00 - 11:20	<b>Coffee break</b>		

11:20 - 12:45	<b>Session 13: Upscaling CO<sub>2</sub> electrolyzers</b> <i>Chair: D. Vermaas</i>	<b>Session 14: Capacitive deionization and supercapacitors</b> <i>Chair: J. Dykstra</i>	<b>Session 15: PEM fuel cells</b> <i>Chair: A. Forner-Cuenca</i>
11:20 - 11:45	683 M. Koper, Advances and challenges in understanding the electrocatalytic conversion of carbon dioxide to fuels	197 A. Forse, Charging Mechanisms and Dynamics in Supercapacitors from NMR Spectroscopy	425 Y. Bultel, Fault detection and identification for Polymer Electrolyte Membrane Fuel Cell
11:45 - 12:00	288 T. Breugelmans, Engineering an industrial CO <sub>2</sub> electrolyzer	364 T. Centeno, Revisiting biomass wastes based-activated carbons in supercapacitors: Volumetric performance	565 J. Mališ, Optimization of the PEM fuel cells MEA preparation by depositing ultrasound dispersed catalytic ink on the membrane surface
12:00 - 12:15	312 L. Baumgartner, Scale-up limitation of gas diffusion electrodes for CO <sub>2</sub> conversion	301 U. Hellriegel, Energy efficient desalination with membrane capacitive deionization (MCDI): findings of theoretical and pilot studies	530 E. Tardy, Modeling of the two-phase transport in PEM fuel cell
12:15 - 12:30	611 M. Vranckaert, Up-scaling a zero-gap CO <sub>2</sub> electrolyzer beyond the pilot scale	270 J. Vos, Ion-Dependent Capacitive Deionization with Porous Carbon Electrodes	286 M. Carvela, Effect of operation temperature on the performance of Hydrogen-Chlorine PEM Fuel Cells
12:30 - 12:45	278 B. Endrődi, Up-scaling zero gap continuous-flow electrolyzer cells for the electrochemical reduction of carbon-dioxide	87 C. Linnartz, Particle Interaction in Slurry Electrodes Influencing the Charge Transport in Flow-Electrode Capacitive Deionization	25 M. Bermúdez Agudelo, Challenges in developing tubular high-temperature proton exchange membrane fuel cells (HT-PEM-FCs)
12:45 - 14:00	<b>Lunch</b>		
14:00 - 14:40	Plenary: K. Chan, The role of double layer charging in electrochemical CO <sub>2</sub> reduction		
14:40 - 15:40	<b>Session 16: Advances in CO<sub>2</sub> electroreduction - II</b> <i>Chair: A. Cornell</i>	<b>Session 17: Electrochemical technologies for the environment - I</b> <i>Chair: S. Ucar</i>	<b>Session 18: Electrocatalysis and electrochemical technologies - I</b> <i>Chair: B. Mei</i>
14:40 - 14:55	616 L. Legrand, Toward market implementation of CO <sub>2</sub> electrochemical reduction to formic acid	542 F. Miao, Tween 80 enhanced electrochemical remediation of phenanthrene contaminated groundwater containing high chloride content	612 D. Budáč, Conductivity of LSM-YSZ layer for thickness of active electrode zone identification
14:55 - 15:10	602 K. Petrov, Using bi-layer membranes to prevent drying-out during CO <sub>2</sub> Electrolysis	459 L. Svecova, Is electro-assisted leaching a feasible option for the recovery of trace elements from municipal solid waste incinerator bottom ash?	193 T. Bystron, Anodic Oxidation of Iodobenzene Derivatives
15:10 - 15:25	405 H. Guzmán, Electroreduction of carbon dioxide on Cu-based mixed-metal oxide catalysts: tuning of syngas composition	303 J. Hives, Ferrates(VI) and Environment	98 A. Raman, Electrolytic gas bubble evolution on a hydrophobic cavity
15:25 - 15:40	258 B. De Mot, The importance of water management in Zero-Gap CO <sub>2</sub> Electrolyzers		
15:40 - 16:00	<b>Coffee break</b>		

16:00 - 17:25	<b>Session 19: Progress in electrocatalysis and electrocatalytic materials</b> <i>Chair: K. Bouzek</i>	<b>Session 20: Electrochemical recovery of raw materials</b> <i>Chair: D. Vermaas</i>	<b>Session 21: Electro-membrane and capacitive processes for advanced separation</b> <i>Chair: M. Biesheuvel</i>	<b>Session 22: Electrochemical engineering for CO<sub>2</sub> capture</b> <i>Chair: M. Tedesco</i>
16:00 - 16:25	682 X. Su, Electrochemical engineering of redox-active systems for materials processing and selective separations	31 M. Hatzell, Photocatalytic nitrogen fixation: Prospects for Distributed Fertilizer Production	681 M. Elimelech, Nanopore-Based Power Generation from Salinity Gradient: Why It Is Not Viable	490 T. Hatton, Electrochemically Modulated Mitigation of Acid Gas Emissions
16:25 - 16:40	413 G. Leftheriotis, Development of photoelectrochromic windows with improved optical and electrical performance	592 M. Rodrigues, Minimal Bipolar Membrane Cell Configuration for Scaling Up Ammonium Recovery	557 L. Monat, Electrodialysis processes for minimizing waste production in phosphoric acid plants	598 R. Sharifian, Harvesting CO <sub>2</sub> from the ocean for circular electrochemical carbonate mineralization
16:40 - 16:55	235 D. Pant, Development and upscaling of gas diffusion electrodes for wastewater treatment and electrosynthesis of chemicals	568 T. Kim, Proton-mediated redox couple to enable ammonia removal and recovery	442 T. Chen, A feasibility study of hybrid capacitive-electrodialysis deionization system for wastewater reuse in the high-tech industrial park	494 Q. Shu, Combined electrochemical desorption of CO <sub>2</sub> and recovery of alkaline sorbent for direct air capture
16:55 - 17:10	159 K. Baitalow, Switchable Oxygen Depolarized Cathodes in flexible Chlor-Alkali Electrolysis	462 L. Bonin, Resource-efficient lithium and sodium recovery from brines using membrane electrolysis	336 A. Lissaneddine, Electrosorption using new biosourced porous electrode material for phenolic compounds removal and valorization – Electrochemical engineering aspects	
17:10 - 17:25		281 F. Lopicque, Beneficiation of jarosite waste assisted by electrochemical operations		

## Day 3: Wednesday 16 June

09:20 - 10:00	Plenary: M. Rodrigo, The binomial Technology Readiness Level / Environmental Electrochemical Engineering: where are we and where are we going?			
10:00 - 11:00	<b>Session 23: Advances in ion transport modelling</b> <i>Chair: M. Tedesco</i>	<b>Session 24: Electrochemical technologies for the environment - II</b> <i>Chair: I. Sirés Sadornil</i>	<b>Session 25: Bioelectrochemistry for energy conversion and resource recovery - I</b> <i>Chair: A. ter Heijne</i>	
10:00 - 10:15	574 M. Biesheuvel, The dynamics of combined ion transport and electrode reactions – Revisiting Bard, Faulkner, and Vetter	367 M. Ingelsson, Utilizing Polarity Reversal in Electrocoagulation to Reduce Electrode Passivation and Enhance Treatment Performance	478 J. Rodríguez, On the behaviour of low-cost MFC: The Contribution of Porous Support Materials	
10:15 - 10:30	471 S. Özkul, Modelling ion transfer through ion exchange membranes in electrodialysis for multi-ionic solutions	285 M. Muñoz Morales, Development of jet electro-absorbers for the treatment of organochlorinated wastes	102 C. Borsje, The granular capacitive moving bed reactor for the scale up of bioanodes	
10:30 - 10:45	453 R. Müller, Modeling electrode-electrolyte interfaces: The differential capacitance of polycrystalline surfaces and non-constant susceptibility	170 H. Bergmann, Electrochemical Treatment of Spent Wire Drawing Solutions	26 S. de Smit, Boosting a biocathode by analysis: the invasive effects of cyclic voltammetry on microbial electrosynthesis	
10:45 - 11:00	339 J. Dykstra, Proton transport across anion exchange membranes in electrochemical systems	121 K. Denk, Electrochemical treatment of membrane concentrates		

11:00 - 11:20	<b>Coffee break</b>		
11:20 - 12:45	<b>Session 26: Water electrolysis and fuel cells - III</b> <i>Chair: T. de Groot</i>	<b>Session 27: Advances in capacitive electrodes for selective ion removal</b> <i>Chair: S. Ucar</i>	<b>Session 28: Bioelectrochemistry for energy conversion and resource recovery - II</b> <i>Chair: B. Hamelers</i>
11:20 - 11:45	600 I. Banerjee, Technology development of water electrolyser design in applied & fundamental domain	88 E. Guyes, Long-lasting, monovalent-selective capacitive deionization electrodes	680 A. ter Heijne, Understanding and influencing biological conversions with electrodes
11:45 - 12:00	420 S. Weusten, Improved reactor design using 3D printed electrolyzers	609 A. Arulrajan, Understanding pH changes during long-term operation of Membrane Capacitive Deionization (MCDI)	599 M. Mascia, Modelling of a Single Chamber Bio-Electrochemical Cell for Wastewater Treatment and Clean Energy Production
12:00 - 12:15	207 M. Tsampas, Solid electrolyte based photoelectrochemical cells for solar hydrogen production	276 J. Lado, Performance Analysis of a Capacitive Deionization Stack Equipped with Graphite Felt 3D Composites Electrodes	375 M. Elzinga, Microbial reduction of organosulfur compounds in bioelectrochemical systems
12:15 - 12:30	194 N. Ivanova, Some specific operating features of PEMFC with binary fuel at low temperatures	124 K. Singh, Tunable Ion Selectivity in Capacitive Deionization with Prussian Blue Analogues	
12:30 - 12:45	108 M. Prokop, Interaction of H <sub>3</sub> PO <sub>3</sub> with Pt in concentrated H <sub>3</sub> PO <sub>4</sub> electrolyte at elevated temperatures		
12:45 - 14:00	<b>Lunch</b>		
14:00 - 14:40	<b>Plenary: MZ. Bazant, Learning the Physics of Batteries from Image Data</b>		
14:40 - 15:40	<b>Session 29: Electrocatalysis and electrochemical technologies - II</b> <i>Chair: R. van de Sanden</i>	<b>Session 30: Electrochemical technologies for the environment - II</b> <i>Chair: T. Sleutels</i>	<b>Session 31: Fast-tracking electrochemical innovations &amp; matchmaking</b> <i>Chair: M. de Graaff</i>
14:40 - 14:55	101 A. Ashaju, Electrocatalytic Reaction Driven Flow	615 J. Su, Electrochemical Reduction of Nitrate over Bimetallic Catalysts in Aqueous Solutions: Effect of crystal structure and surface morphology	From Lab to Plant: Accelerating implementation of electrochemical technologies <i>Organized by VoltaChem</i>
14:55 - 15:10	15 J. Sun, Enhanced fouling mitigation of conductive membrane electrode by electro-repulsion and in-situ electro-cleaning in an electro-membrane reactor (EMR)	338 F. Durán, Development of a scrubbing processes using absorbents-electrolytes to the elimination of volatile organic contaminants	<i>Keynote speakers: R. Latsuzbaia, A. Lüken</i> <i>Panel discussion with R. Latsuzbaia, A. Lüken, B. Bakker</i>
15:10 - 15:25		331 Y. Shih, Electrochemical reduction of nitrate over Cu and Pd-Cu nanocatalysts as affected by crystalline morphology and facet	
15:25 - 15:40			
15:40 - 16:00	<b>Coffee break</b>		
16:00 - 17:30	<b>Matchmaking session</b> <i>Powered by New Energy Coalition</i>		

## Day 4: Thursday 17 June

09:20 - 10:00	<b>Plenary: G. Kelsall, Material recovery from end-of-life batteries</b>		
10:00 - 11:00	<b>Session 32: Novel electrodes for OER/ORR</b> <i>Chair: T. de Groot</i>	<b>Session 33: Electrochemical processes for sustainable energy and production of chemicals</b> <i>Chair: M. Tedesco</i>	<b>Session 34: Electrochemical processes applications</b> <i>Chair: B. Mei</i>
10:00 - 10:15	564 J. Geppert, Monitoring Catalytic Changes by Microkinetic Modelling of the Oxygen Evolution Reaction	614 L. Ma, Transport and adsorption of organic micropollutants in reverse electro dialysis	573 V. Kyriakou, Redox Exsolution: A Novel Bottom-Up Catalyst Preparation Method for Efficient Electrochemical Energy Applications
10:15 - 10:30	461 M. Carda, Identification of rate determining step for OER and ORR in solid oxide electrochemical cell	562 R. Kunkel, Electrochemical Vanillin Reduction in a Flow Reactor: A Route to Biobased Polymers	540 P. Saha, Comparison of electrochemical and vacuum ultraviolet (VUV)-based oxidation processes for cooling tower blowdown treatment -a case study
10:30 - 10:45	192 V. Gueskine, Oxygen reduction reaction at conducting polymer electrodes: Insights from DFT modeling	103 E. Andreou, Simulation Modelling for Sustainable Large-scale Electroforming	468 R. Latsuzbaia, Electrochemical process development for production of bio-based maleic acid
10:45 - 11:00		41 C. Simões, Multistage reverse electro dialysis effect for energy generation	63 J. White, Mass transport effects on the electrooxidation of glycerol on electrodeposited palladium-nickel catalysts
11:00 - 11:20	<b>Coffee break</b>		
11:20 - 13:00	<b>Session 35: Electrochemical technologies for the environment - III</b> <i>Chair: J. Dykstra</i>	<b>Session 36: Electrocatalysis and electrochemical technologies - III</b> <i>Chair: M. Zheludkevich</i>	
11:20 - 11:45	359 I. Sirés Sadornil, Changing the configuration of an air-diffusion cathode reactor to operate Fenton-based treatments of organic pollutants in continuous mode	215 R. van de Sanden, Plasma activated electrolyser for nitrogen fixation by water	
11:45 - 12:00	333 F. Adnan, Influence of Micrometric Inter-Electrodes Distance and Water Hardness on Mineral Scaling at Electrode Surface during Electrochemical Advanced Oxidation Process	209 O. Cornejo, Design and characterization of a novel flow-through electrochemical reactor for hydrogen peroxide electrosynthesis directed to the incineration of organic compounds by electrochemical advanced oxidation processes	
12:00 - 12:15	199 J. Llanos, Advanced treatments for depleting non-polar organochlorine pesticides from concentrated sludges	189 K. Wenderich, Towards anodic H <sub>2</sub> O <sub>2</sub> production as a profitable commodity chemical in PEC water splitting	
12:15 - 13:00	<b>CWME Award Ceremony</b>		
13:00 - 14:00	<b>Lunch</b>		
14:00 - 14:40	<b>Award lecture: C. Comninellis, New views in the anodic oxidation of organics The Electrochemical Oxygen Transfer Reactions (EOTR)</b>		
14:40 - 15:10	<b>ESEE 2021 Awards and Closing Ceremony</b>		
15:10 - 16:00	<b>Coffee break</b>		



	<b>Tutorials</b>
16:00 - 16:45	M. Koper, Molecular theory of the Butler-Volmer rate law
16:45 - 17:30	M. Biesheuvel, Ions in water near and in electrodes. Mass transport and reaction modeling as simple as possible

## Plenary: Life's emergence: an early success story of electrochemical free energy conversion

*W. Nitschke (Centre National de la Recherche Scientifique, France)*

The prevailing narrative for life's origin assumes the spontaneous self-organization of prebiotic organics into primitive protocells. This scenario obviously has a severe problem with the 2nd Law of Thermodynamics. However, so has life in general ... An examination of how present life on this planet negotiates the requirements imposed by the 2nd law comes up with a simple answer: it's all about electrochemistry! Redox gradients provide the ultimate source of free energy ( $\Delta G$ ) and electrochemical processes of all sorts drive the buildup of order (processes and structures) fuelled by the influx of such (redox) free energy ( $\Delta H \rightarrow -T\Delta S$ ). The unicity of this principle in extant life suggests it to also have been operating at life's emergence and to even represent the ultimate reason for why life has emerged in the first place. The fundamental (redox) free energy converters of extant life will be presented and potential prebiotic precursors of these processes will be discussed.

## 555 | Mitigation of capacity and efficiency loss in vanadium redox flow batteries: mathematical model and experimental validation

*Martin Bureš (University of Chemistry and Technology, Prague), Jiří Charvát (University of Chemistry and Technology, Prague), Petr Mazúr (University of Chemistry and Technology, Prague), Juraj Kosek (University of Chemistry and Technology, Prague), Jaromír Povedič (University of West Bohemia)*

### Abstract

Vanadium redox flow battery (VRFB) is a potential electrochemical energy storage solution for residential accumulation and grid stabilization. The long-term durability, non-flammability and high efficiency represent the main advantages of the technology. The ion-exchange membrane, an essential component of the battery stack, is largely responsible for the efficiency and capacity fade caused by reversible asymmetric cross-over of vanadium ions and a solvent. To mitigate capacity and efficiency fade in VRFBs, we developed a mathematical model and validated it against experimental measurements. Our model simulates the performance of a VRFB under seven sets of conditions, differing in current, membrane, initial volume, initial concentration, storage tank connection (hydraulic shunt) and periodic remixing. Furthermore, it describes dynamic charge-discharge cycling with vanadium permeation, osmotic pressure and flux and electrode reactions. The hydraulic shunt connection of storage tanks (HS) appears to be the most promising, reducing capacity losses by 69 % over 150 cycles. Moreover, combining methods showed that using AEM with HS and remixing can store and release up to 80 % more energy than a standard VRFB using CEM. Our model not only optimizes the construction and maintenance of VRFBs but can also be easily adapted to other types of RFB.

### Biography: Martin Bureš

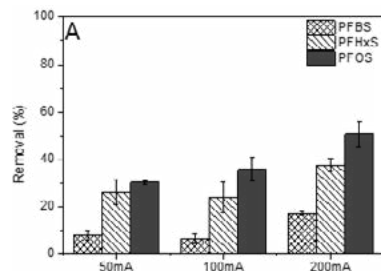
My name is Martin Bures and I received master's degree in 2020 in Chemical engineering from University of chemistry and technology in Prague. I am studying Ph.D. in chemical engineering under supervision of Prof. Kosek and Dr. Mazur. I am specialized in mathematical modelling of electrochemical systems. Currently, my research is specialized into the mitigation and optimization of a Vanadium redox flow batteries and the optimization of the carbon felt electrode.

### 516 | Graphene Sponge Electrodes for Electrochemical Degradation of Perfluoroalkyl Substances (PFAS)

Nick Duinslaeger (Catalan Institute for Water Research (ICRA)), Jelena Radjenovic (ICRA)

#### Abstract

In this work, electrochemical degradation of six model perfluoroalkyl substances is studied using graphene sponge anode and cathode. Electrooxidation experiments were conducted in a one-pass mode using a flow-through cell equipped with a B-doped graphene sponge anode and an Ndoped graphene sponge cathode. A systematic experimental study was conducted to evaluate the influence of (i) the applied current density,  $j_{app}$ , (ii) the carbon chain length and functional group and (iii) the hydrodynamic conditions, in terms of flowrate. In the experiments conducted under environmentally relevant conditions and using low-conductivity supporting electrolyte ( $\sim 1$  mS cm<sup>-1</sup>), and low initial PFASs concentration (0.2  $\mu$ M), we demonstrated the enhanced removal % with increased applied anodic current and hydraulic residence time, with up to 62.4% removal for PFOS in one-pass, continuous mode of operation. We observed decreased removal % of PFASs with shortening of the chain length in the order: C8>C6>C4, for both PFASs as PFCAs, as well as preferential removal of PFASs over PFCAs over the applied current range. Hereby we demonstrate the possibility of PFAS removal using low-cost carbon-based electrode materials.



#### Biography: Nick Duinslaeger

In 2012, Nick graduated from the Catholic University of Leuven, Belgium, where he obtained his Master of Science in Catalytic Science and Technologies at the faculty of Bioscience Engineering. He started working as a project manager for Veolia Water Technologies, whereafter he joined Médecins Sans Frontières as a Technical Referent Environmental Health where he was involved in several of MSF's operational research projects. From September 2019 onward, Nick has been working at the Catalan Institute for Water Research, where his research is focused on the development of novel anode materials and design of nanoelectrochemical systems for the degradation of PFASs.

### 164 | Spatially resolved model for oxygen reduction reaction in porous gas-diffusion electrodes

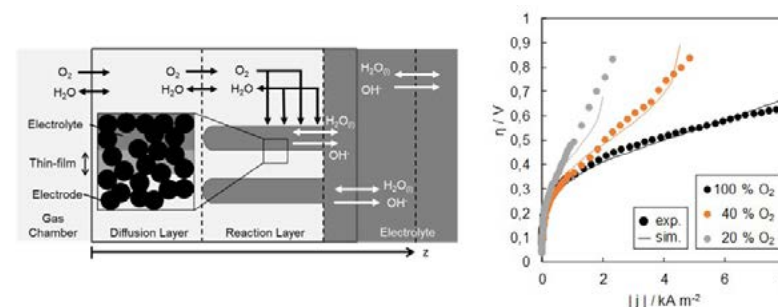
David Franzen (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr. 17, 38678 Clausthal-Zellerfeld), Barbara Ellendorff (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr. 17, 38678 Clausthal-Zellerfeld), Jens Osiewacz (Clausthal University of Technology, Institute of Chemical and Electrochemical Process Engineering, Leibnizstraße 17, D-38678 Clausthal-Zellerfeld, Germany), Thomas Turek (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr. 17, 38678 Clausthal-Zellerfeld)

#### Abstract

Gas diffusion electrodes (GDE) are key components in the modern chlor-alkali electrolysis process. By introducing the oxygen depolarized cathode (ODC), the electrical energy consumption is reduced by up to 30 % compared to the state-of-the-art membrane process. In order to investigate the complex interaction of transport and reaction inside the ODC a stationary mathematical model is developed, including transport processes in gas and liquid phase as well as electrochemical reaction kinetics (Fig. 1, left). While earlier publications [1] underestimated transport processes, the improved version of the thin-film flooded-agglomerate (TFFA) model considers the electrolyte transport and electrowetting phenomena adequately. Additionally the electrolyte properties and resulting process parameters, such as oxygen solubility and diffusion coefficients, are spatially resolved.

The model is validated by experiments made with a custom build test setup under industrial process conditions (80 °C, 30 wt.% NaOH). A wide range of process conditions (temperature, pressure, oxygen- and electrolyte concentration) can be adjusted and stationary conditions at the GDE are guaranteed during long-term measurements. Measured and simulated overvoltages are in good agreement (Fig. 1, right).

[1] S. Pinnow, N. Chavan, T. Turek (2011) Thin film flooded agglomerate model for silver-based oxygen depolarized cathodes. J Appl Electrochem 41(9): 1053–1064. doi: 10.1007/s10800-011-0311-8



#### Biography: David Franzen

In 2017 Master's degree in Chemical Process Engineering at Clausthal University of Technology. Subsequently employed as research assistant at the Institute of Chemical and Electrochemical Process Engineering within the framework of the DFG Research Group 2397: Multiscale analysis of complex three-phase systems: Oxygen reduction at gas diffusion electrodes in aqueous electrolyte.

### 340 | Half-Cell Monitoring at All-Vanadium-Flow-Batteries (VFB)

*Claudia Weidlich (DECHEMA-Forschungsinstitut), Theresa Haisch (DECHEMA-Forschungsinstitut), Hyunjoon Ji (DECHEMA-Forschungsinstitut), Nicky Bogolowski (DECHEMA-Forschungsinstitut)*

#### Abstract

Vanadium flow batteries (VFB) are a promising technology to store renewable energy. For an efficient operation, the reliable detection of the state of charge (SOC) of the battery during its charging and discharging is essential. At a VFB test station monitoring methods as measuring potential, density <sup>[1]</sup> and UV-Vis spectrometry have been investigated for the *in situ* determination of SOC as well as detection of electrolyte crossover. Measuring the open circuit potential (OCP) at the battery half-cells is a simple and cost-effective method [1]. OCP Monitoring has been tested concerning the applicability for continuous determination of SOC and identification of electrolyte crossover <sup>[2]</sup>. This work is done within the joint research project “DegraBat”. “DegraBat” is funded by the German Federal Ministry of Economic Affairs and Energy (BMWi) within the government’s funding initiative energy storage.

#### References

[1] State of charge monitoring of vanadium redox flow batteries using half cell potentials and electrolyte density, S. Ressel, F. Bill, L. Holtz, N. Janshen, A. Chica, C. Weidlich, T. Struckmann, Journal of Power Sources, Volume 378, 28 February 2018, Pages 776-783

[2] Monitoring the state of charge of all-vanadium redox flow batteries to identify crossover of electrolyte, T. Haisch, H. Ji, C. Weidlich, Electrochimica Acta, <https://doi.org/10.1016/j.electacta.2019.135573>

#### Biography: Claudia Weidlich

I am working at the Electrochemistry group of the DECHEMA-Forschungsinstitut since 1998. Actually I am team leader Redox- flow batteries.

### 430 | Electrochemical Disinfection of E. Coli with Reduced Graphene Oxide Foam Electrodes

*Giannis-Florjan Norra (1Catalan Institute for Water Research (ICRA), Scientific and Technological Park of the University of Girona, c/Emili Grahit 101, 17003 Girona, Spain 2University of Girona (UdG), Plaça Sant Domènec, 3 Edifici Les Àligues, 17004 Girona), Luis Baptista Pires (1Catalan Institute for Water Research (ICRA), Scientific and Technological Park of the University of Girona, c/Emili Grahit 101, 17003 Girona, Spain 2University of Girona (UdG), Plaça Sant Domènec, 3 Edifici Les Àligues, 17004 Girona), Carles Borrego (Catalan Institute for Water Research (ICRA)), Jelena Radjenovic (ICRA)*

#### Abstract

Electrochemical treatment is a promising and emerging method of (waste)water disinfection, which has the advantage of not requiring any chemical addition to operate. In electrochemical disinfection processes, the production of oxidants (disinfectants) may occur directly by water discharge (i.e., hydroxyl radicals, ozone), dissolved species (i.e., active chlorine or hydrogen peroxide via oxygen reduction), or anode dissolution (i.e., ferrate). When chlorine is present in water, the active species can enhance the disinfection capacity, but this has the drawback of generating toxic disinfection by-products (DBPs). In this study we achieved up to 3 log removal of *E. Coli* in the absence of chlorine species, using graphene-based anode and cathode in a one pass mode. Graphene foam electrodes were prepared using a simple, low-cost method. The main advantage of the prepared graphene foams is that they did not produce any chlorine, chlorate or perchlorate, which is one of the main limitations in electrooxidation of chloride-containing water. Higher log removal of *E. coli* can be easily achieved by coupling several reactor modules in line. The developed electrode materials are extremely promising as they can provide successful disinfection without forming toxic DBPs, thus opening the door for future electrochemical water treatment applications.

#### Biography: Giannis-Florjan Norra

Dipl.–Ing. Giannis-Florjan Norra obtained his Chemical Engineering Diploma from the National Technical University of Athens (NTUA), Greece in 2015. While preparing his thesis, he was also working as a research assistant in the “Biotechnology Laboratory” of NTUA. He also worked as a research assistant in the Thermodynamics and Transport Phenomena Laboratory of the School of Chemical Engineering (NTUA) from November 2016 till April 2017. Giannis joined the Catalan Institute for Water Research in May, 2018. His research is focused on the development of flow-through packed bed electrochemical reactors for the treatment of persistent contaminants and disinfection.

## 204 | Effect of Carbon Dioxide from Ambient Air on Alkaline Exchange Membranes for Fuel Cells

Fabian Kubanek (Technische Universität Braunschweig), Avital Zhegur-Khais (Technion - Israel Institute of Technology), Dario R. Dekel (Technion - Israel Institute of Technology), Ulrike Krewer (Technische Universität Braunschweig)

### Abstract

Alkaline Exchange membrane fuel cells (AEMFC) are attractive because less costly materials can be used. Currently, the operation with ambient air remains an unsolved challenge. In AEMFC, hydroxide ions migrate from the cathode to the anode. In contact with ambient air,  $\text{CO}_2$  dissolves in the membrane and reacts with hydroxide ions to carbonates. Under equilibrium conditions, hydroxide is almost completely replaced by carbonates. Experiments show that this causes a drastic decline in cell performance because of lower ion mobility in the membrane and additional kinetic overpotentials<sup>1</sup>. During cell operation, the carbonation is partly reversed by an electrochemical decarbonation process<sup>2</sup>. In this contribution, a model is presented and validated which describes the carbonation and decarbonation of anion exchange membranes. The model is parameterized with experimental data from various membrane types, and the effect of membrane properties on carbonation and decarbonation is analyzed in detail. Based on the model, desirable properties of carbonation-tolerant membranes are derived. Our work is an important step towards designing and operating AEMFC that deliver high performance with ambient air.

### Reference

- <sup>[1]</sup> Y. Zheng et al., *Energy Environ. Sci.*, 12, 9, 2806–2819, 2019.  
<sup>[2]</sup> U. Krewer et al., *Electrochim. Acta*, 263, 433–446, 2018.

### Biography: Fabian Kubanek

Fabian Kubanek is a PostDoc at the Institute of Energy and Process Systems Engineering at Technische Universität Braunschweig. He obtained his diploma in industrial engineering in 2013. His research focuses on experimental and modelbased analysis of reaction kinetics and mass transport in microbial fuel cells, alkaline exchange membrane fuel cells, electrolyzers and metal-airbatteries.

## 231 | Optimisation of flow field designs for vanadium redoxflow batteries

Eva Prumbohm (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstraße 17, 38678 Clausthal-Zellerfeld, Germany and Research Center Energy Storage Technologies, Am Stollen 19a, 38640 Goslar, Germany), Gregor D. Wehinger (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstraße 17, 38678 Clausthal-Zellerfeld, Germany and Research Center Energy Storage Technologies, Am Stollen 19a, 38640 Goslar, Germany), Thomas Turek (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstraße 17, 38678 Clausthal-Zellerfeld, Germany and Research Center Energy Storage Technologies, Am Stollen 19a, 38640 Goslar, Germany)

### Abstract

Vanadium redox-flow batteries allow to store large amounts of electrical energy. Flow fields can be employed to decrease the pressure losses, homogenise the flow distribution, and improve the mass transport from the fluid bulk to the carbon electrode surface<sup>[1]</sup>. However, a modification of the flow field influences the different effects by a varying degree. Therefore, to find a reasonable compromise, a flow field design optimisation is carried out by means of computational fluid dynamics simulations. Starting point is a typical interdigitated flow field design with square shaped channels and a carbon felt electrode, which is characterised by its porosity and permeability<sup>[2]</sup>. The effect of the mass transport on the concentration change is included by considering the limiting current density. For the flow field design process, the objective criteria such as maximum limiting current density and minimum pressure drop are defined and several geometric parameters are changed, see Figure1. Finally, novel flow field designs are achieved, which stand out by their high performance.

### Reference

- [1] M.R. Gerhardt, A.A. Wong, M.J. Aziz, *J Electrochem Soc* 165 (2018) A2625–A2643.  
<https://doi.org/10.1149/2.047181jes> .  
 [2] E. Prumbohm, G.D. Wehinger, *Chem Ing Tech* 91 (2019) 900–906.  
<https://doi.org/10.1002/cite.201800164> .

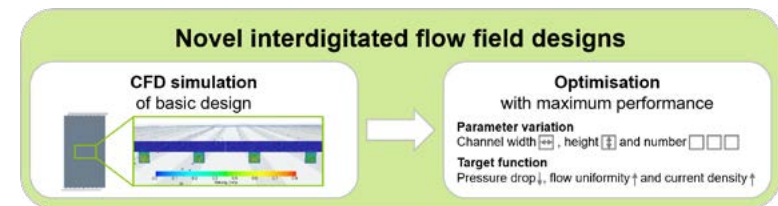


Figure1: Overview of simulation and optimisation process.

### Biography: Eva Prumbohm

Eva Prumbohm is a PhD student at the Institute of Chemical and Electrochemical Process Engineering at Clausthal University of Technology in Germany. In her field of research, she models vanadium redox-flow batteries at the cell and system level based on CFD simulations. Additionally, experimental studies such as optical measurements are carried out. Her research interests cover flow field designs, electrode characteristics and mass transport. Beforehand, she studied process engineering at Clausthal University of Technology at the master level and mechanical engineering at Technische Universität Braunschweig at the bachelor level.

### 248 | Photo-assisted electrochemical disinfection of hospital urines using a novel flow-through reactor

Miguel Herraiz Carbone (University of Castilla-La Mancha), Salvador Cotillas (University of Castilla-La Mancha), Engracia Lacasa (University of Castilla-La Mancha), Pablo Cañizares (University Hospital Complex of Albacete), Caridad Sainz de Baranda (University Hospital Complex of Albacete), Manuel A. Rodrigo (University of Castilla-La Mancha), Cristina Sáez (University of Castilla-La Mancha)

#### Abstract

In last years, the use of electrochemical technologies for wastewater disinfection has gained increasing attention because they are environmentally-friendly processes with high efficiencies for microorganisms' removal. Within the effluents that present high levels of pathogens, hospital urines can be considered as one of the main sources of these microorganisms. Hence, the disinfection of these effluents has become a new challenge to face for wastewater treatment. With this background the aim of the present work is to evaluate the electrochemical and photoelectrochemical disinfection process of hospital urines with a flow-through reactor. A three-dimensional titanium mesh coated with Teflon and carbon black that maximize the hydrogen peroxide generation is used as cathode material. The influence of the current density has been also studied on the process to assess a complete disinfection, avoiding the formation of undesirable by-products.

#### Acknowledgements

This work has been supported by Junta de Comunidades de Castilla-La Mancha (JCCM), European Union (European Regional Development Fund) and Ministry of Science and Innovation through the projects SBPLY/17/180501/000396 and PID2019-110904RB-I00. The Spanish Ministry of Science, Innovation and Universities is also acknowledged for the "Juan de la Cierva-Incorporación" post-doctoral grant (IJC2018- 036241-I) awarded to Dr. Salvador Cotillas.

#### Biography: Miguel Herraiz Carbone

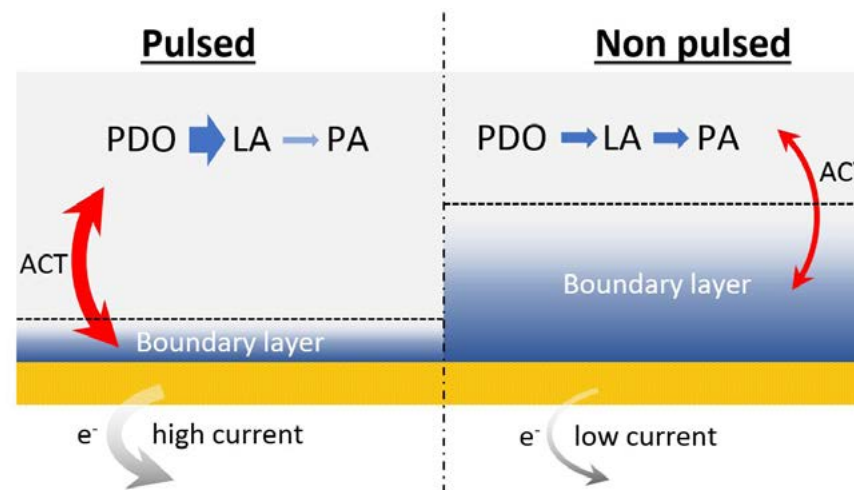
Mechanical engineer from the University of Castilla La Mancha in 2013, Master in industrial mechanics in 2014 from the Carlos III University of Madrid and Master in Industrial Engineering from the University of Castilla La Mancha in 2018. I have developed my research activity at the Laboratory of Electrochemical and Environmental Engineering, belonging to the TEQUIMA Research Group of the University of Castilla La Mancha from 2018. It has been focused on the Environmental Applications of Electrochemical Engineering and, currently, I am a PhD student. Specifically, I am working in the application of novel electrochemical reactors for hospital urines disinfection.

### 114 | Overcoming mass transport limitations in electrochemical reactors with a pulsating flow electrolyzer

Elena Perez Gallent (TNO), Carlos Sánchez Martínez (TNO), Leon Geers (TNO), Susan Turk (TNO), Roman Latsuzbaia (TNO), Earl Goetheer (TNO; TUDelft)

#### Abstract

Electrochemical processes are a promising technology for the industrial production of chemicals. One of the major drawbacks of electrochemical systems is the low mass transfer of reactants towards the active surface area of the electrode. In this study, an approach is presented to enhance the mass transfer and increase the overall performance of the reactions. The strategy comprises the introduction of a pulsed electrolyte flow in the electrochemical flow cell. This pulsating behavior results in an improved mass transfer of electroactive species due to a higher instantaneous velocity driven by the pulsations. Though the net residence time of the reactants will not be altered due to the pulsation, the resulting enhancement of mass transfer leads to an increase of the conversion. The oxidation of 1,2-propanediol to lactic acid and pyruvic acid mediated by 4-acetamido-(2,2,6,6-tetramethylpiperidin-1-yl)oxidanyl (ACT-TEMPO) was chosen to study the influence of the pulsed flow. Under the pulsating regime, a yield increase of lactic acid of a factor of two and a 15-20% gain in selectivity to a total of 95% towards lactic acid can be achieved by tuning the process parameters.



#### Biography: Carlos Sánchez Martínez

Carlos Sánchez Martínez studied chemical engineering at University of Alicante in Spain; then he moved to the Netherlands to start the PDEng program in Process and Product Design in TU Eindhoven. He then joined TNO Energy Transition in 2018 and started working in the Sustainable Process and Energy Systems department as a chemical process research scientist. He based his research on the development of models and elaboration of technoeconomical analysis for electrochemical processes. Besides, he participates in studies for CO<sub>2</sub> mitigation strategies with industrial partners.

## 206 | Investigations on the vanadium ion reaction kinetics on single carbon fibre electrodes

Isabelle Kroner (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr. 17, 38678 Clausthal-Zellerfeld, Germany), Maik Becker (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr. 17, 38678 Clausthal-Zellerfeld, Germany), Thomas Turek (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr. 17, 38678 Clausthal-Zellerfeld, Germany)

### Abstract

The vanadium redox flow battery (VFB) is a promising energy storage system, due to its durability and safety. However, the kinetics of the vanadium ion reactions have not yet been investigated in detail. Previous studies on these kinetics were only performed on model electrodes such as platinum<sup>[1]</sup>.

For understanding the interplay between electrolyte and electrode, investigations on commercial materials, such as porous carbon felts are necessary. However, the low conductivity of the electrolyte results in inhomogeneous current density distributions in the porous electrode, which makes an exact determination of kinetic parameters very difficult.

Therefore, we used microelectrodes (similar to those of Miller et al.<sup>[2]</sup>) with single fibres from commercial electrode materials to determine the rate constants and reaction orders of the vanadium kinetics under realistic conditions. Thus, precise kinetic parameters can be determined, which can be used in electrode models and might also help to improve the materials.

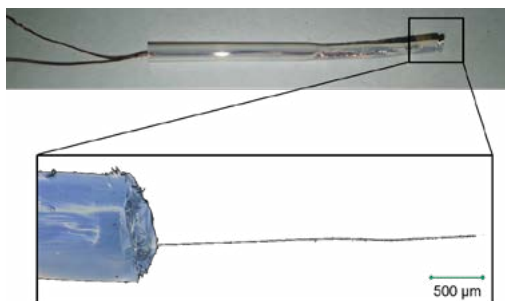


Figure 1: Carbon fibre microelectrode.

### Reference

[1] W. Wang, X. Fan, Y. Qin, J. Liu, C. Yan, C. Zeng, *Electrochimica Acta* 283 (2018) 1313–1322. <https://doi.org/10.1016/j.electacta.2018.07.071>

[2] M.A. Miller, A. Bourke, N. Quill, J.S. Wainright, R.P. Lynch, D.N. Buckley, R.F. Savinell, *J. Electrochem. Soc.* 163 (2016) A2095-A2102. <https://doi.org/10.1149/2.1091609jes>

### Biography: Isabelle Kroner

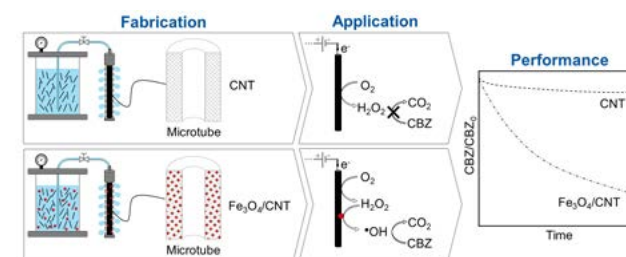
In 2017 Isabelle Kroner completed her master's degree in chemical engineering at Clausthal University of Technology. Since then, she has been a research assistant at the Institute of Chemical and Electrochemical Process Engineering. Her field of research are detailed investigations on the kinetics over porous carbon electrodes in vanadium redox flow batteries.

## 162 | Fe<sub>3</sub>O<sub>4</sub>-incorporated carbon microtubes as efficient electrodes for the degradation of persistent pollutants at neutral pH

Mojtaba Mohseni (RWTH Aachen University, Aachener Verfahrenstechnik-Chemical Process Engineering), Kristof Demeestere (Ghent University), Gijis Du Laing (Ghent university), Süleyman Yüce (RWTH Aachen University, Aachener Verfahrenstechnik-Chemical Process Engineering), Matthias Wessling (RWTH Aachen University, Aachener Verfahrenstechnik-Chemical Process Engineering and DWI - Leibniz-Institute for interactive materials e.V.)

### Abstract

Fenton-based electrochemical advanced oxidation processes are regarded as promising techniques for degrading persistent pollutants such as pharmaceuticals. Among them, heterogeneous electro-Fenton (HEF) in comparison to homogeneous electro-Fenton (EF) has gained lots of attention since HEF widens the operational pH window from strongly acidic to circumneutral pH values by immobilizing the catalyst on the electrode surface. Nevertheless, the primary challenge is to develop an electrode through a single-step synthesis method, which possesses high electrical conductivity, large surface area, easy catalyst incorporation, and adequate mechanical and chemical stability. This study introduces novel carbon microtubes (CMTs) made of commercial carbon nanotubes (CNTs) and Fe<sub>3</sub>O<sub>4</sub> nanoparticles. In CMTs, the CNT matrix firmly embeds the Fe<sub>3</sub>O<sub>4</sub> nanoparticles without any chemical bonds. CMTs functioned as efficient electrodes for the degradation of carbamazepine (CBZ), a frequently detected pharmaceutical in water bodies, at pH 7. A current density of 0.9 mA cm<sup>-2</sup> was sufficient to degrade 94±3 % of CBZ-- resulting in specific energy consumption (SEC) of 0.015 kWh g<sup>-1</sup>CBZ, which is by far the lowest value reported in the literature. The introduced synthesis method bridges the scale of confinement control of nano-sized catalyst particles and macroscale product geometry, offering an easy scale-up through the numberingup of CMTs.



### Biography: Mojtaba Mohseni

- IRANIAN
- NOV 2016 – NOW: Joint Ph.D. researcher (Marie-Curie Fellow) in Chemical Process Engineering (RWTH Aachen University in Germany and Ghent University in Belgium) Topic: “Fenton-based technologies for micropollutants removal.”
- SEP 2011- JAN 2014: M.Sc. in Chemical Engineering (Sharif University of Technology in Tehran, Iran)
- PUBLICATIONS:
  - Mohseni, Mojtaba, et al. “Freestanding PAC/CNT microtubes remove sulfamethoxazole from water through a temperature-assisted cyclic process.” *Journal of hazardous materials*\_ 392 (2020).
  - Mohseni, Mojtaba, et al. “The highest inhibition coefficient of phenol biodegradation using an acclimated mixed culture.” *Water Science and Technology*\_ 73.5 (2016): 1033-1040.

**372 | Impact of batteries ageing on their state of security**

Xavier Fleury (Univ. Grenoble Alpes, CEA, LITEN, DEHT), Sylvie Genies (Univ. Grenoble Alpes, CEA, LITEN, DEHT), Loic Lonardoni (Univ. Grenoble Alpes, CEA, LITEN, INES), Sebastien Dumenil (Univ. Grenoble Alpes, CEA, LITEN, INES), Pierre Xavier Thivel (Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, LEPMI)

**Abstract**

Lithium-ion technology meets the needs of multiple applications thanks to its undeniable assets. However, the state of security of lithium batteries as they age is still an important issue. The safety behaviour of two types of LFP batteries has been tested after ageing under calendar or cycling conditions during overcharge tests. Prior to the overcharge test, the cells were equipped with surface temperature sensors and strain gauges and then charged with a C/10 rate at 100% of SOC. Then an overcharge at 2C up to 2 x U<sub>max</sub> was performed in a safety box. *Post-mortem* analyses of fresh, aged and overcharged cells have been carried out. It has been shown that the gaseous emissions associated with the degradation of the SEI and the reactivity of the lithiated graphite with the electrolyte result in an increase in internal pressure of the cell and a higher temperature for the batteries aged under calendar mode. Normally, safety devices allow gas venting and current interruption to reduce the risk of thermal runaway. However, it has been observed that the interruption of the current is not systematic after the opening of the security vent paving the way for a hazardous scenario for the user.

**Biography: Pierre Xavier Thivel**

Pierre-Xavier Thivel, Assistant Professor at Université Grenoble-Alpes and researcher at the Laboratory of Electrochemistry and Physicochemistry of Material and Interfaces (LEPMI UMR 5279).

Scientific domain: Chemical engineering & electrochemical engineering.

Scientific topics :

- CONVERSION AND ELECTROCHEMICAL ENERGY STORAGE PROCESSES : Diagnostic and the characterization of electrochemical processes (Fuel cell, Batteries...), Development of innovating tools (acoustic emission, electrochemical noise, ...) and thermal and mechanical measurement for electrochemical system,
- RECYCLING PROCESSES OF ELECTROCHEMICAL GENERATORS AND ENVIRONMENTAL ENGINEERING: Development of hydrometallurgical processes for metal recovery of electrochemical system (fuel cell and batteries).

**618 | M. Suss, Co-generation of electricity and desalted water using chemical energy**

*Matthew Suss, Technion Israel Institute of Technology, Israel*

**Abstract**

Desalination technologies are often classified by the form of their energetic input, such as mechanical energy (reverse osmosis), thermal energy (distillation), or electrical energy (electrodialysis, capacitive deionization). Here, we present the development of a nascent technology which desalinates water using instead chemical energy, in the form of redox-active chemicals. As we will show, simultaneous to desalination, such a cell also outputs net electricity. We will describe both the fundamental thermodynamics of such a system, which predicts the maximum available electricity during desalination of seawater of up to ~25 kWh per m<sup>3</sup> of clean water, and our work in developing a proof-of-concept experimental system based on hydrogen-oxygen chemistry. The latter cell, which we term a "Desalination Fuel Cell", delivered up to 10 kWh/m<sup>3</sup> of electricity while desalinating synthetic seawater (30 g/L NaCl). We will present the outlook on this technology, which can co-generate electricity and clean water using a single cell.



## 51 | Rethinking Alkaline Water Electrolysers

*J.W. (Willem) Haverkort (Delft University of Technology, Process & Energy, 3mE)*

### Abstract

Despite more than a century of industrial water electrolysis, there are still large gaps in literature in the understanding and optimization of alkaline water electrolysers. This talk will discuss several recent innovative approaches to improve electrolyser design :

- Are electrodes most effectively stacked in a conventional sandwich structure? A 'checkerboard' pattern can make for more compact electrolysers. <sup>[1]</sup>
- Does a zero-gap design minimize the ohmic losses? We discuss the counter-intuitive finding that a small gap between the electrode and diaphragm can actually significantly reduce the cell voltage.
- Is a diaphragm required to keep oxygen and hydrogen apart? Using a modest electrolyte flow through porous electrodes, gases can be effectively and energy-efficiently be separated <sup>[2]</sup>

We finally discuss the recent finding that electro-osmotic flows can arise inside the diaphragm, transporting dissolved oxygen towards the hydrogen side <sup>[3,4]</sup>.

### References

- [1] Rajaei, H., & Haverkort, J. W. (2020). Compact monopolar electrochemical stack designs using electrode arrays or corrugated electrodes. *Electrochimica Acta*, 332, 135470.
- [2] Rajaei, H., Rajora, A., & Haverkort, J. W. (2021). Design of membraneless gas-evolving flow-through porous electrodes. *Journal of Power Sources*, 491, 229364.
- [3] Haverkort, J. W., & Rajaei, H. (2020). Electro-osmotic flow and the limiting current in alkaline water electrolysis. *Journal of Power Sources Advances*, 6, 100034.
- [4] Haverkort, J. W. (2020). Modeling and Experiments of Binary Electrolytes in the Presence of Diffusion, Migration, and Electro-Osmotic Flow. *Physical Review Applied*, 14(4), 044047.

### Biography: J.W. (Willem) Haverkort

Dr. ir. J.W. (Willem) Haverkort is a tenure track assistant professor at Delft University of Technology. After studying Applied Physics in Delft (*cum laude*), with honours track in theoretical physics at UvA), a PhD in computational and theoretical magnetohydrodynamics of nuclear fusion plasmas (CWI/DIFFER), he worked at the Shell Amsterdam laboratories on a wide variety of industrial fluid mechanics research problems. Back in Delft, he focuses on theory, modelling, and experiments of multiphase fluid mechanics in electrochemical systems in general and porous electrodes in particular. His main applications are water electrolysis, CO<sub>2</sub>-reduction, and redox flow batteries.

## 563 | Concentration and Velocity Profiles in a Polymeric Lithium-ion Battery Electrolyte

*Hans-Georg Steinrück (Universität Paderborn), Christopher Takacs (SLAC National Laboratory), Michael Toney (UC Boulder)*

### Abstract

Predictive understanding of ion and mass transport in electrolytes is at the heart of electrochemistry. The goal is to accurately simulate the performance of an electrochemical cell, for which the concentration-dependent transport coefficients of a given electrolyte must be known. These include the transference number, which is an important metric to energy and power density of batteries. Nevertheless, researchers still argue about transference number values, even in baseline electrolytes.

We developed an alternative approach towards determining transport coefficients [EES 13, 4312 (2020)]. Specifically, we measured microscopic and macroscopic physical properties of electrolytes upon cell polarization in Li/electrolyte/Li cells, combined this with concentrated solution theory continuum modelling, and rationalized our findings with microscopic insight from molecular dynamics simulations. We utilized a well-studied benchmark model system electrolyte consisting of LiTFSI and PEO. Under constant voltage polarization, we directly measured the velocity associated with electrolyte and ions via heterodyne synchrotron X-ray photon correlation spectroscopy (XPCS), and the TFSI-concentration gradient via X-ray absorption microscopy. The significance of our results lies in the unification of microscopic and macroscopic predictions from simulation with experimental measurements as well as the self-consistent determination of a concentration-independent transference numbers of approximately 0.2.

### Biography: Hans-Georg Steinrück

After receiving his PhD in physics in 2015, Hans-Georg Steinrück spent five years at SLAC National Laboratory (USA) as a postdoctoral fellow and associate staff scientist, where he investigated energy storage and transformation materials using synchrotron radiation. In 2020, he became an Assistant Professor in the Department of Chemistry at the University of Paderborn. His research interests include interfaces, electrochemistry, energy storage, self-assembly, synchrotron techniques, and clean water.

## 570 | Energy consumption for fluoride removal using constant current operated capacitive deionization system

Yusufu Abeid Chande Jande (Water Infrastructure and Sustainable Energy Futures (WISE-Futures) centre, Nelson Mandela African Institution of Science and Technology, Arusha)

### Abstract

The cities found in the Rift Valley (Arusha being among of them) has challenges with high fluoride concentration in water; above the 1.5 ppm (World Health Organization recommended limit). Different studies are being conducted to find out the best technology for fluoride removal. Some technologies are currently being in use: adsorption (using bone char) and reverse osmosis (RO). However, these technologies have some shortcomings. Adsorption technique has poor regeneration ability and also is not suitable for large scale operation; RO system usually needs more energy to remove fluoride. This study reports the use of capacitive deionization (CDI) for fluoride removal; the model by Jande and Kim (2013) on constant current operation of CDI system is being used. Three cases with different concentration have been examined: 15 ppm, 10 ppm, and 5 ppm; resulted in energy consumption of 4.8 Wh/m<sup>3</sup>, 3.2 Wh/m<sup>3</sup>, and 1.6 Wh/m<sup>3</sup>.

Case No.	CDI feed (ppm)	flow rate to CDI (mL/s)	Amount of water produced in one cycle (litres)	Cycle time (h)	Purity of water (ppm)	Energy consumption (Wh/m <sup>3</sup> )
1)	15	20	580	16.1	0.052	4.8
2)	10	20	870	24.2	0.023	3.2
3)	5	20	1740	48.3	0.0057	1.6

### Biography: Yusufu Abeid Chande Jande

Yusufu Abeid Chande Jande completed PhD at Hanyang University in 2015, Mechanical Engineering Department, South Korea and MSc and BSc in Mechanical Engineering from Middle East Technical University, Ankara, Turkey. He is currently lecturing in the Department of Materials and Energy Science and Engineering ([www.nmaist.ac.tz](http://www.nmaist.ac.tz)); and also the Deputy Centre Leader of Water Infrastructure and Sustainable Energy Futures centre ([www.wisefutures.ac.tz](http://www.wisefutures.ac.tz)). Yusufu is interested in capacitive deionization for desalination and CO<sub>2</sub> capture and rapid prototyping specifically in producing uniformly porous and graded porous structures using selective laser sintering (SLS) and producing composite materials from porous structures manufactured using SLS.

## 607 | Controlling gas bubble nucleation and release in alkaline electrolysis

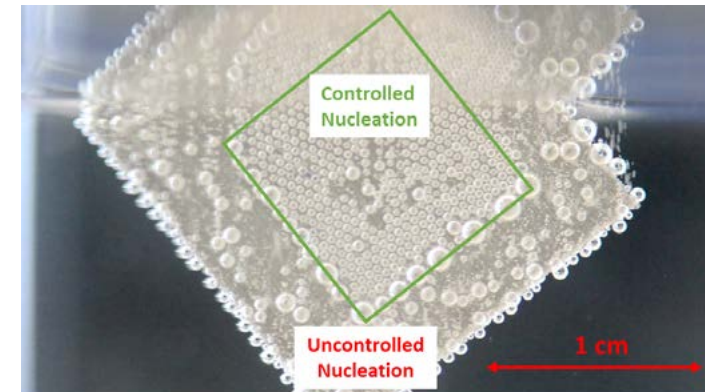
Jorrit Bleeker (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands), Oliver Westerman (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands), David Vermaas (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands)

### Abstract

Renewable hydrogen production is expected to play a key role in the energy transition. Alkaline electrolysis uses abundant transition metal electrodes to achieve high activity for hydrogen and oxygen evolution, making it a cost-effective water electrolysis technique. The main drawback of alkaline electrolyzers is the low energy efficiency at high current densities (>0.2 A/cm<sup>2</sup>). A large fraction of the energy losses can be attributed to gas bubbles, that partially block the electrode surface and reduce the conductivity of the electrolyte. Controlled nucleation and efficient removal of gas bubbles is therefore crucial to fully optimize electrolyzers.

We developed a cheap and easy method to control gas bubble nucleation by partially coating a Nickel electrode with a water repelling shoe spray. The control of local hydrophobicity opens up route to control the number, detachment size and location of the gas bubbles (see figure). In addition, we developed a method to remove these bubbles by periodic variations in the pressure, or a "pressure swing".

The combination of the controlled gas bubble nucleation and the pressure swing allows control over the bubble-related resistance in the system. We demonstrate that higher average current densities can be obtained at the same voltage.



### Biography: Jorrit Bleeker

In 2018 I graduated from the MSc Chemical Engineering programme at the Delft University of Technology, doing a thesis work on a novel heatpower technology using redox flow batteries under supervision of David Vermaas.

From 2018 until March 2020 I worked as a Process safety engineer for PM Group Global in Cork, Ireland, mainly designing pressure safety valves.

In April 2020 I came back to Delft to do a PhD under supervision of David and Ruud van Ommen, working on improving the mass transfer and energy efficiency of gas evolving electrolysis techniques.

## 524 | Effect of fast charging on Lithium plating and SEI growth

Nireas Rigos (German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Stuttgart), Timo Danner (German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Stuttgart), Simon Hein (German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Stuttgart), Arnulf Latz (German Aerospace Center (DLR), Institute of Engineering Thermodynamics, Stuttgart)

### Abstract

Metallic lithium deposition (Plating) and continuous Solid Electrolyte Interface (SEI) growth are two dominant degradation mechanisms in Lithium-ion battery electrodes. Particularly in fast-charging applications, the identification and prediction of those complex electrochemical processes is crucial for the development of efficient and long-lasting batteries as well as suitable charging protocols. Thereby, especially the interplay between SEI growth and Li-Plating over the lifetime of the battery is not yet properly understood.

The present work employs a model-based approach to study the aging phenomena on the surface of graphitic anode materials during high-current cell operation. For this purpose, a combined surface model is formulated, which couples the aforementioned anode aging mechanisms and is able to relate them to the local conditions at the graphite surface. The coupled description is based on models for lithium plating and SEI growth recently developed in our group. Furthermore, the model is implemented in the electrochemical simulation framework BEST for 3D micro-structure resolved simulations, which will allow us to correlate electrode microstructure with degradation processes, especially for fast charging applications.

### Biography: Nireas Rigos

2020-04 – PHD POSITION, German Aerospace Center @ Helmholtz Institute Ulm  
 present Institute of Engineering Thermodynamics, Computational Electrochemistry  
 Research topic: Modeling and simulation of degradation mechanisms at high-energy anodes  
 2014 – CHEMICAL ENGINEERING DIPLOMA, National Technical University of Athens  
 2019 Concentration: “Process Engineering”  
 Thesis: “Mapping of the operation of a chemical vapor deposition reactor”  
 2018-08 – ERASMUS INTERNSHIP, Helmholtz- Zentrum Dresden-Rossendorf  
 2018-12 Publication: V. Vishwakarma, N. Rigos, M. Schubert, U. Hampel, “Efficiency estimation of tray columns based on flow profiles and vapor-liquid equilibrium characteristics of binary mixtures” <https://doi.org/10.1021/acs.iecr.9b04915>

## 548 | Electrochemical removal of amphoteric ions

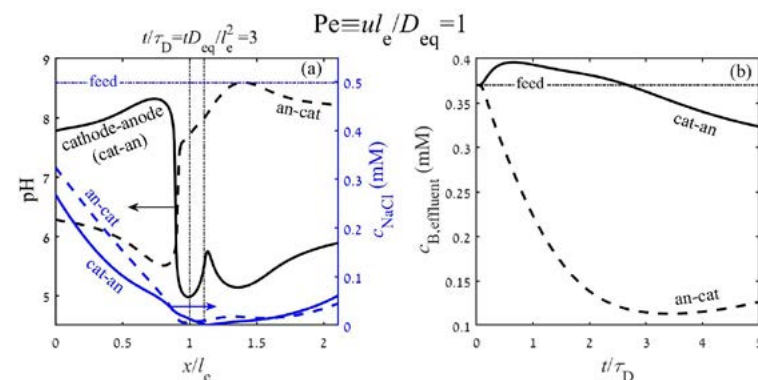
Amit N. Shocron (Faculty of Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel), Eric N. Guyes (Faculty of Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel), Maarten Biesheuvel (Wetsus), Huub Rijnaarts (Wageningen University), Jouke Dykstra (Wageningen University), Matthew Suss (Faculty of Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel)

### Abstract

Several harmful or valuable ionic species in water are amphoteric, i.e., their charge depends on the electrolyte pH. As separation processes for ions removal from water are often based on ionic charge, effective removal of these species is challenging, and the electrolyte pH may have to be adjusted to achieve separation.

Capacitive deionization (CDI) is an emerging technique for water treatment and desalination, based on electrosorption of salt ions into microporous electrodes. CDI cells show large internally-generated pH gradients during operation, and thus CDI can potentially remove amphoteric ions without adjusting the feed pH and in an economic manner. Here, we present a novel theoretical framework predicting the adsorption of amphoteric ions in micropores, while considering pH-dependent chemical surface groups in the micropores, ion transport in the macropores, and local electrolyte pH. Moreover, we account for association and dissociation reactions of amphoteric ions in the electrolyte.

We demonstrate that such a model enables deep insight into factors affecting amphoteric ion electrosorption, and we compare with experimental results of the removal of boric acid. The figure below presents pH and salt concentration profiles, along with effluent boron concentration, for flow-through CDI cells with the cathode placed upstream (cat-an) or downstream (an-cat).



### Biography: Amit N. Shocron

I am a Ph.D. candidate in the Department of Mechanical Engineering in the Technion - Israel Institute of Technology, and I have graduated B.Sc. Summa cum Laude and M.Sc. cum Laude in the same department. I have co-authored 4 published journal papers and have given 4 presentations at international conferences. During my Ph.D. studies, I have been rewarded for academic excellence by Daniel Citation and Jacobs Citation and won a poster prize given by Nature Nanotechnology. Also, I took part in guiding two B.Sc. students, who won a prize for the best poster in the Israel electrochemistry conference.

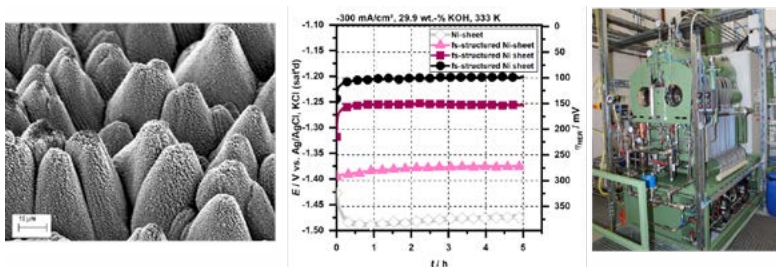
#### 445 | Highly active electrodes for alkaline water electrolysis by femtosecond-laser processing

Thomas Rauscher (Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Branch Lab Dresden, Winterbergstraße 28, 01277 Dresden, Germany), Christian Bernäcker (Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Branch Lab Dresden, Winterbergstraße 28, 01277 Dresden, Germany), Eike Hübner (Fraunhofer Heinrich Hertz Institute, Am Stollen 19H, 38640 Goslar, Germany), Wolfgang Schade (Fraunhofer Heinrich Hertz Institute, Am Stollen 19H, 38640 Goslar, Germany AND TU Clausthal, Institute of Energy Research and Physical Technologies, Am Stollen 19B, 38640 Goslar, Germany), Thomas Weißgärber (Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Branch Lab Dresden, Winterbergstraße 28, 01277 Dresden, Germany), Lars Röntzsch (Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Branch Lab Dresden, Winterbergstraße 28, 01277 Dresden, Germany)

##### Abstract

In this contribution, we report on a novel femtosecond (fs) laser process that is applied to produce electrodes for alkaline water electrolysis.<sup>[1]</sup> The fs-process induces the roughening of the substrate surface which is characterized by periodical features, resembling fine cones. The process parameters were adjusted to improve the activity for both hydrogen and oxygen evolution reaction. The fs-laser structured substrate materials were analyzed with respect to the morphology, composition and electrochemical properties. The electrochemical activity of Ni alloys was strongly improved in iterative steps and a periodic cone-like structure decorated with a porous oxide surface layer showed the highest activity. The best electrodes revealed an HER overpotential value of 105 mV at -300 mA/cm<sup>2</sup>. Beside the excellent robustness and the high catalytic activity, the electrodes can be processed very fast in one step without any post processing. Finally, a benchmark test was made in a commercial electrolyzer (BAMAG-technology). Therefore, flat perforated Ni-sheets (0.25 m<sup>2</sup>) were processed. Commercial Raney-Ni electrodes were used as benchmark. The results revealed that the fs-laser structured electrodes outperform the Raney-Ni electrodes in the test campaign.

<sup>[1]</sup> a) A. Gabler et al. \_Int. J. Hydrogen Energy\_ 2017, 10826; b) T. Rauscher, et al., \_Electrochim. Acta\_ 2017, 1130.



##### Biography: Thomas Rauscher

Thomas Rauscher is a research fellow at the Fraunhofer Institute for Manufacturing Technology and Advanced Materials in Dresden, where he coordinates R&D projects. He graduated from the Technische Universität Dresden with a diploma in material science. Thomas has more than 6 years' experience in research and development for hydrogen and fuel cell technology. In particular, he works on the development of advanced electrode materials for the water electrolysis (10 publications).

#### 449 | From first to second life of lithium-ion batteries study

Pierre Xavier THIVEL (Université Grenoble Alpes), Eddy Coron (CEA), Sylvie GENIES (Univ. Grenoble Alpes, CEA, LITEN, DEHT), Mikaël Cugnet (Univ. Grenoble Alpes, CEA, LITEN, INES)

##### Abstract

Second life of lithium-ion batteries is under investigation because it could be economically and environmentally profitable. However, the second life longevity of electric vehicles aged cells depends on aging parameters, as well as the state of health (SOH) shift point between first and second life. In this study, it has been set to 80%, and two different cycling temperatures applied to two different references of 18650-format cells were tested as a first life aging. Periodical electrochemical check-ups allowed the monitoring of pulse resistance, incremental capacity analysis and electrochemical impedance spectroscopy. At the end of their first life, some cells were dismantled for visual and SEM inspections. It revealed in numerous cases the occurrence of lithium plating at the negative electrode, especially after aging at low temperature. Thicknesses, weights and electrochemical measurements of both electrodes confirmed this observation. Accelerated rate calorimetry (ARC) indicated the thermal safety degradations induced by the lithium plating. Similar aged cells were kept for a softer second life aging, with a reduced cycling rate. The over-aging longevity appeared to be depending on the first life, i.e. on the degradation mechanism. The occurrence of lithium plating seems to be tolerable only if its extension is limited.

##### Biography: Pierre Xavier Thivel

Pierre-Xavier Thivel, Assistant Professor at Université Grenoble-Alpes and researcher at the Laboratory of Electrochemistry and Physicochemistry of Material and Interfaces (LEPMI UMR 5279).

Scientific domain: Chemical engineering & electrochemical engineering.

Scientific topics :

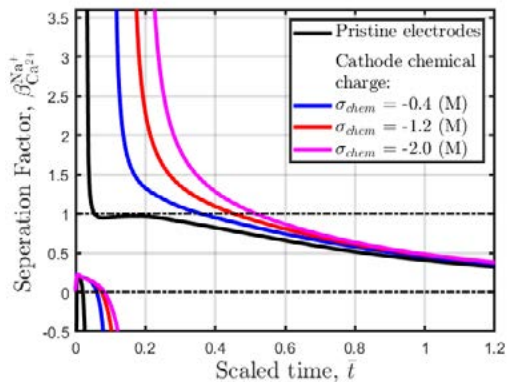
- CONVERSION AND ELECTROCHEMICAL ENERGY STORAGE PROCESSES : Diagnostic and the characterization of electrochemical processes (Fuel cell, Batteries...), Development of innovating tools (acoustic emission, electrochemical noise, ...) and thermal and mechanical measurement for electrochemical system,
- RECYCLING PROCESSES OF ELECTROCHEMICAL GENERATORS AND ENVIRONMENTAL ENGINEERING: Development of hydrometallurgical processes for metal recovery of electrochemical system (fuel cell and batteries).

**527 | Theory of monovalent ion selectivity using porous carbon capacitive deionization electrodes**

Zohar Sahray (Faculty of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel), Amit N. Shocron (Faculty of Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel), Eric N. Guyes (Faculty of Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel), Matthew Suss (Faculty of Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel)

**Abstract**

Capacitive deionization (CDI) is a fast-emerging technology that is commonly applied to water treatment, where a typical CDI cell consists of two microporous carbon electrodes and a dielectric separator. Predicting the storage dynamics of each species for feedwater with mixture of several ions is challenging, as this depends on time, electrode parameters and electrolyte properties. An emerging application for CDI is water treatment for agriculture use, in which it is often important to selectively adsorb sodium and chloride, both monovalent ions, over divalent calcium, magnesium and sulfate ions. To explain different selectivity mechanisms, we developed a transient model for a flow-through electrode CDI cell which includes competing cationic species, ion size effects, and chemically-treated electrodes. We unravel several effects which lead to monovalent selectivity, and suggest a mechanistic explanation. Several factors can be tuned to enhance monovalent selectivity at short charging times, including micropore chemical charge, and anode placement (upstream or downstream). The figure shows the effect of the cathode chemical charge on the separation factor, quantifying the selective adsorption of monovalent ions, where values higher than unity represent monovalent selectivity, and negative values represent desorption. Increasing the cathode’s chemical charge, elongates the period where the electrodes are monovalent selective.



**Biography: Zohar Sahray**

I am a M.Sc. student and I have graduated B.Sc. cum Laude in Mechanical Engineering in the Technion - Israel Institute of Technology. I have given 2 presentations related to capacitive deionization in the Israel electrochemistry conference where we won poster prize (as a coauthor) and in the final B.Sc. project where I won poster prize. I also took part in the Formula Student competitions where I presented the design considerations of the vehicle in 5 competitions.

**326 | An analytical model for liquid and gas diffusion layers in electrolyzers and fuel cells**

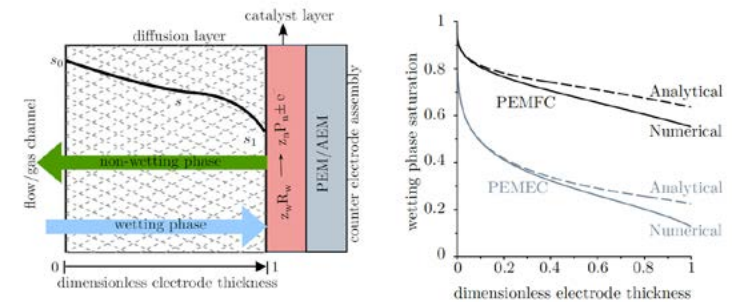
Aviral Rajora (Delft University of Technology, Process Energy, 3mE), J.W. (Willem) Haverkort (Delft University of Technology)

**Abstract**

Knowing the reacting phase saturation is essential to characterize the performance of the diffusion layer. We consider the multiphase transport inside a diffusion layer and present a fully analytical model to calculate the saturation as shown in the (right) figure. The model can be applied generally to both electrolyzers and fuel cells, as long as the gas and liquid phases move in opposite directions, as shown in the (left) figure. The model includes the effect of pore-size distribution through the Brooks-Corey relation<sup>1</sup> and uses the relative permeability approach<sup>2</sup>. We provide analytical expressions for limiting currents associated with flooding or reactant starvation as well as for overpotentials in fuel cells and electrolyzers. In this talk, we provide examples for hydrophobic and hydrophilic diffusion layers used in hydrogen fuel cells and water electrolyzers and show that currently available diffusion layers are well designed. We also analytically show why the MPL should be made thinner than the GDL and why most of the transport losses occur in the catalyst layers.

**References**

- <sup>1</sup> R. H. Brooks, A. T. Corey, Hydraulic properties of porous media, Hydrology papers (Colorado State University); no. 3.
- <sup>2</sup> S. Litster, N. Djilali, Two-phase transport in porous gas diffusion electrodes, 2005.



(Left): Schematic of the electrochemical cell showing multiphase transport in a diffusion layer. (Right): Analytical and numerical saturation profiles for both fuel cells and electrolyzers.

**Biography: Aviral Rajora**

Aviral Rajora is a PhD student at the Process and Energy Laboratory, Delft University of Technology in the area of multiphase flow modelling in porous electrodes. He is currently focussing on full-cell modelling of CO<sub>2</sub> electrolyzers. Aviral received his Bachelor’s degree in Mechanical Engineering from the Indian Institute of Technology, Varanasi (IITBHU), India in 2013, and a Masters in Solid and Fluid Mechanics from the Delft University of Technology in 2017 studying the heat transfer in particle-laden turbulent channel flow.

## 42 | Enhancing the part-load range of alkaline water electrolyzers by model-based optimization

Jörn Brauns (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr. 17, 38678 Clausthal-Zellerfeld), Thomas Turek (Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr. 17, 38678 Clausthal-Zellerfeld)

### Abstract

Alkaline water electrolysis is a promising technology to use higher amounts of renewable energies within the framework of the energy turnaround. Excessive wind or solar power can be converted into hydrogen, which is usable as an almost emission-free fuel in the transport sector or for the decarbonization of industrial processes. The part-load range of conventional alkaline water electrolyzers is restricted, because the gas impurity can reach the lower explosion limit (LEL) when only few energy is available <sup>[1]</sup>. This contribution shows how alkaline water electrolyzers should be designed and why dynamic operation strategies are important to enhance the part-load range. A mathematical process model is used, which extends an existing approach <sup>[2]</sup>. The model is validated by experiments in a lab-scale electrolyzer. The renewable power profile in Fig. 1 can be used to determine optimal system dimensions and operation strategies.

### References

- [1] P. Trinke, P. Haug, J. Brauns, B. Bensmann, R. Hanke-Rauschenbach, T. Turek, J. Electrochem. Soc. 165 (2018) F502–F513.  
 [2] P. Haug, B. Kreitz, M. Koj, T. Turek, Int. J. Hydrogen Energy 42 (2017) 15689–15707.

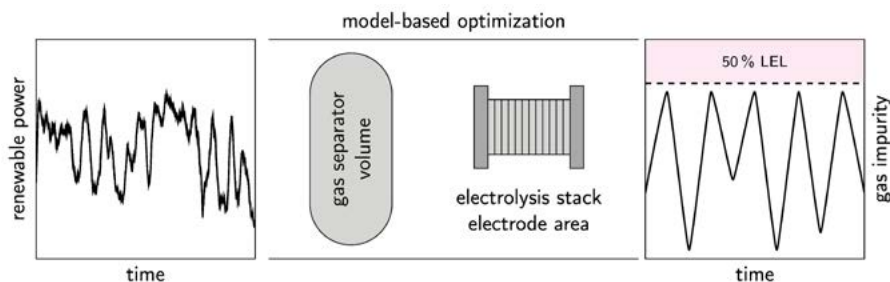


Fig. 1: Schematic of model-based optimization. A fluctuating power profile can be used to determine optimal system dimensions and suitable dynamic operation strategies.

### Biography: Jörn Brauns

Jörn Brauns is a PhD student at the Institute of Chemical and Electrochemical Process Engineering at Clausthal University of Technology. His research focuses on the dynamic operation of alkaline water electrolysis including experimental and theoretical studies about gas purity and overall system performance in combination with renewable energies. He is also researching in the field of electrode development. Previously, he studied chemical process engineering at Clausthal University of Technology.

## Plenary: Electrochemical ammonia synthesis

M. Wessling (RWTH Aachen University, Chemical Process and Product Engineering)

Electrification of chemical processes is currently envisioned as a solution to render today's fossil based chemical industry more sustainable. The membrane-based chlor-alkali electrolysis serves as a proof that such electrified conversion processes are technically and economically viable. The market for water electrolysis currently grows rapidly. The next grand challenge is the reduction of carbon dioxide which is currently in the developmental stage. A new frontier in its infant state is the reduction to ammonia.

Some techno-economical analysis demonstrated that the electrochemical ammonia synthesis may be viable<sup>1</sup>, and publications have reported catalytic systems indicating that nitrogen can indeed be transformed to ammonia with electrochemically produced proton. A very critical review and evaluation of such published data suggests however that reported Faradaic efficiencies and production rates of many reported systems may be systematically flawed by experimental inaccuracies<sup>2</sup>. Here we present recent new data on electrochemical ammonia synthesis which would pass the criteria of above paper as “plausible yet unlikely to be practical” to “highly plausible and promising”.

The presentation describes methodology to develop a new electrocatalytic system<sup>3</sup> combining

- a ruthenium/ carbon black gas diffusion electrode (Ru/CB GDE)
- with a three compartment flow cell, enabling solid–liquid–gas catalytic interfaces for the highly efficient Ru-catalyzed eNRR.

The electrolyte optimization and the Ru/CB GDE development through the hydrophobicity, the Ru/CB loading, and the post-treatment have revealed the crucial contribution of interfacial N<sub>2</sub> transportation and local pH environment.

This work highlights the critical role of design and optimization of the GDE-flow cell combination in order to overcome the experimental difficulties addressed in<sup>2</sup>

### References

1. Kugler, K., Ohs, B., Scholz, M. & Wessling, M. Towards a carbon independent and CO<sub>2</sub>-free electrochemical membrane process for NH<sub>3</sub> synthesis. Phys. Chem. Chem. Phys. 16, 6129–6138 (2014).
2. Choi, J. et al. Identification and elimination of false positives in electrochemical nitrogen reduction studies. Nat. Commun. 11, 1–10 (2020).
3. Wei, X., Pu, M., Jin, Y. & Wessling, M. Efficient Electrocatalytic N<sub>2</sub> Reduction on Three-Phase Interface Coupled in a Three-Compartment Flow Reactor for the Ambient NH<sub>3</sub> Synthesis. ACS Appl. Mater. Interfaces 13, 21411–21425 (2021).

## 558 | Development of aqueous redox flow batteries based on organic electroactive compounds

*Petr Mazúr (University of Chemistry and Technology, Prague, Dep. of Chemical Engineering), Michaela Mikešová (University of Chemistry and Technology, Prague, Dep. of Chemical Engineering), Jaroslav Kvcála (University of Chemistry and Technology, Prague, Dep. of Organic Chemistry), Zuzana Burešová (University of Pardubice, Inst. of Organic Chemistry and Technology), Milan Klikar (University of Pardubice, Inst. of Organic Chemistry and Technology), Filip Bureš (University of Pardubice, Inst. of Organic Chemistry and Technology), Lubomír Kubáč (Centre for Organic Chemistry, Rybitví)*

### Abstract

Vanadium redox flow batteries, with several MWhscale installations worldwide<sup>[1]</sup>, proved to be a safe, reliable and long-lasting energy storage technology. However, high and fluctuating price of vanadium stimulates the seek for alternative active compounds. Organic redox couples are particularly attractive<sup>[2, 3]</sup> as their relevant properties can be tailored by modification of their chemical structure. Moreover, they can be produced at high volumes and low costs e.g., from oil residues.

In our contribution, we present the development of aqueous organic redox flow battery based on bipyridine and anthraquinone compounds including following steps: i) synthesis of novel active compounds and their basic characterization; ii) study of chemical/electrochemical stability under RFB operation including NMR post-mortem analysis; iii) optimization of electrolyte formulation with respect to relevant properties (solubility, ionic conductivity, viscosity); iv) performance and stability evaluation of electrolytes in RFB cells.

### Acknowledgments

The work was supported from European Regional development Fund-Project "Organic redox couple based batteries for energetics of traditional and renewable resources (ORGBAT)" No.CZ.02.1.01/0.0/0.0/16\_025/0007445.

### Biography: Petr Mazúr

Post-doc researcher focusing on research and development of redox flow batteries for stationary energy storage based on various chemistries such as vanadium, organic and metal-air.

## 595 | Novel porous TiOx anode materials for the removal of organic pollutants from water

*Jing Ma (Laboratoire Géomatériaux et Environnement), Clément Trelu (Laboratoire Géomatériaux et Environnement), Nihal Oturan (Laboratoire Géomatériaux et Environnement), Mehmet A. Oturan (Laboratoire Géomatériaux et Environnement)*

### Abstract

Electrochemical advanced oxidation processes are efficient water treatment technologies, though problems such as mass transfer were observed with conventional dense electrodes. Implementation of porous electrodes in flowthrough configuration has gained lots of attention in recent years. This study focused on the development of TiOx coated Ti foam and 100% TiOx foam and membranes with various synthesis methods, in collaboration with Saint-Gobain Research Provence. All Ti/TiOx foam performed better than dense Ti/TiOx for the removal of various model pollutants (paracetamol, tetracycline) and probe molecules (oxalic acid for direct electron transfer, terephthalic acid for hydroxyl radicals). Quenching experiments highlighted the predominance of hydroxyl radical mediated oxidation and direct electron transfer. Active chlorine mediated oxidation was also important in chloride-containing medium, but sulfate radical mediated oxidation was not significant (even in 50 mM Na<sub>2</sub>SO<sub>4</sub>). The data obtained in terms of degradation and mineralization effectiveness were discussed according to the different material characteristics. Comparison was also performed between batch and flow-through configurations. Results showed that pore structure has a very different impact on electro-oxidation effectiveness for batch and flowthrough configurations, depending on mass transfer conditions. Results obtained emphasized that the different electrodes and configurations might have different applications (diluted effluents, concentrated effluents).

### Biography: Jing Ma

Jing Ma is a doctoral student at Université Gustave Eiffel, Laboratoire Géomatériaux et Environnement, under the supervision of Dr. Clément Trelu and Prof. Mehmet A. Oturan. Her doctoral research mainly focuses on application of porous Ti/TiOx materials in water remediation, understanding of the reaction mechanisms, lifetime evaluation of Ti/TiOx materials and potential ways of extending lifetime of the materials. She has started her PhD in December 2019. For her PhD program, she works in collaboration with an industrial partner for electrode manufacturing.

**263 | Sustainable Syngas Production in Power-to-X Technologies**

L. G.J. (Bert) de Haart (Institute of Energy and Climate Research, Fundamental Electrochemistry (IEK- 9), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany), Rüdiger Eichel (Institute of Energy and Climate Research, Fundamental Electrochemistry (IEK-9), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany / Institute of Physical Chemistry, RWTH Aachen University, 52074 Aachen, Germany)

**Abstract**

The development of sustainable production processes and the use of regenerative resources based on “Power-to-X” (P2X) technologies is a promising approach for reducing climate-damaging CO<sub>2</sub> emissions in industrial processes. In P2X a major role is foreseen for syngas production by high-temperature co-electrolysis of carbon dioxide and water vapour. Syngas, a mixture of hydrogen and carbon monoxide, is used on a large scale for the production of basic chemicals like ammonia and methanol, but can be used also for the synthesis of synthetic fuels<sup>[1]</sup>. High-temperature Solid Oxide Electrolysis Cells (SOECs) are capable of simultaneous reduction of water vapour and carbon dioxide. In the framework of the German Kopernikus project ‘Power-to-X’ co-electrolysis is investigated and further developed to meet the requirements for the subsequent hydrocarbon synthesis, i.e. ‘tailoring’ of the syngas compositions. Commercially available cells are investigated by the combination of electrochemical methods (current-voltage characteristics, electrochemical impedance spectroscopy) and an all-embracing quantitative product analysis. Experiments under varying conditions (temperature, current density, gas composition) were performed and conclusions about the competitive fundamental reactions have been drawn by comparison in combination with thermodynamic modelling.

**References**

[1] S. Foit, I.C. Vince, L.G.J. de Haart, R.-A. Eichel, *Angew. Chem. Int. Ed.* 56 (2017) 5402-11

**Biography: L.G.J. (Bert) de Haart**

- Master degree in chemistry / State University of Utrecht, The Netherlands (1981)
- PhD in solid state chemistry / State University of Utrecht, The Netherlands (1985)
- Post-Doc, University of Twente, Enschede, The Netherlands (1987-1992)
- Scientist, Forschungszentrum Jülich GmbH, Germany (1992-present)
- Institute of Energy and Climate Research, Electrochemical Process Engineering (IEK-3), (1992-2011)
- Institute of Energy and Climate Research, Fundamental Electrochemistry (IEK-9), (2011-present)
- Recent Research Topic: Electrochemical Energy Storage and Conversion

**380 | Simulation of hydrodynamics, mass transport and current distribution in a Cerium-Vanadium redox flow battery**

Isabel Leon-Sotelo (University of Guanajuato), José L. Nava (University of Guanajuato)

**Abstract**

Redox flow batteries (RFBs) are an excellent candidate for large-scale renewable energy storage. One of the most attractive features is the scaling of power and energy capacity of the battery, which is a function of effective electrode area and electrolyte characteristics<sup>1</sup>. The design of an RFB includes several interrelated factors, such as electrode material, reactor geometry, and the characterization of the reaction environment in terms of fluid flow, electrolyte composition, mass and heat transport, electrode kinetics, and current distributions, in order to find the best operational conditions to reach a suitable energy efficiency<sup>2</sup>. This work deals with the design of a cerium-vanadium RFB (Ce-VRFB); the well-known FM01-LC reactor was used as a flow cell. CFD simulations of single-phase flow within the graphite felt (used as an electrode), mass transport, current distribution, state of charge, and power density were performed. Close agreement between simulations and experimental determinations of mass transport coefficients, state of charge, and power density was attained, as shown in Figure 1. A commercial code to solve the transport equations through the finite element method was employed.

**References**

<sup>1</sup> *A two-dimensional model of the vanadiumcerium redox flow battery.* SMITH, SCOTT, ET AL. 2019, *Electrochimica Acta* 328, p. 135019.

<sup>2</sup> *Mathematical modeling and simulation of the reaction environment in electrochemical reactors.* CATAÑEDA, LOCKSLEY F., ET AL. 2019, *Current Opinion in Electrochemistry* 16, pp. 75- 82.

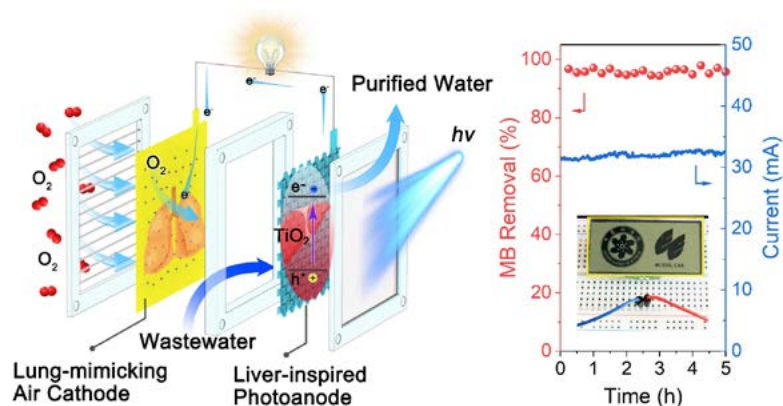


## 502 A biomimetic photocatalytic system for efficient electricity generation from wastewater treatment

Dr. Zhenao Gu (Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences), Prof. Chengzhi Hu (State Key Laboratory of Environmental Aquatic Chemistry, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences)

### Abstract

Energy recovery from wastewater treatment is attracting tremendous research interests since the environmental and energy issues can be simultaneously addressed. Photocatalytic fuel cell (PFC) provides a sustainable way for water purification and electricity generation. Herein, we demonstrated an integrated PFC platform by mimicking the metabolic processes in human body. Inspired by the purification of metabolites in the microstructure of liver lobules, flow-through  $\text{TiO}_2$  photoanode with numerous microchannels was developed. Compared to traditional PFC with planar photoanode, the biomimetic microflow PFC exhibited 3 to 5-fold enhancements in the removal efficiencies of various organic pollutants, including perfluorooctanoic acid, 4-chlorophenol, bisphenol A, methylene blue, and amoxicillin. To mimic the breathing process in alveoli, an ultrathin air cathode was fabricated by sputtering Pt (loading as small as  $0.01 \text{ mg cm}^{-2}$ ) on nanoporous polyethylene film. The construction of this dual-biomimetic PFC system resulted in an open circuit voltage of 0.92 V and a record-high power output of  $500 \mu\text{W cm}^{-2}$  under simulated solar light. The series connection of modularized reactors allowed for the successive purification of wastewater by self-generated electricity. Thus, this work opens up new opportunities of biomimetic photocatalytic system for addressing the water-energy nexus.



### Biography - Zhenao Gu

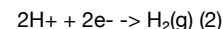
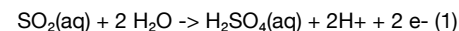
Zhenao Gu obtained his PhD in 2020 from University of Chinese Academy of Sciences under the supervision of Prof. Jiu-hui Qu. He is currently a postdoctoral researcher in the group of Prof. Chengzhi Hu at Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences. His research focuses on the (photo)electrochemical techniques for pollutants removal and energy/resource recovery.

## 256 | Addressing the challenges of the $\text{SO}_2$ depolarized electrolysis at high temperature

Sergio Díaz Abad (University of Castilla La Mancha), Mireya Carvela (University of Castilla La Mancha), Manuel A. Rodrigo (University of Castilla-La Mancha), Justo Lobato (University of Castilla La Mancha)

### Abstract

Among the numerous technologies for hydrogen production, the thermochemical cycles are becoming of great interest as long as the required energy comes from renewable energies. One of them is the Hybrid Sulfur Cycle, where hydrogen is produced in  $\text{SO}_2$  electro-oxidation step according to equations 1 and 2. What makes this cycle a promising technology is the low theoretical cell potential of 0.158 V compared with the standard water electrolysis potential of 1.23 V.



The aim of this work is to develop the technology for increasing the current working temperature used of  $80^\circ\text{C}$  to a range of  $100\text{--}200^\circ\text{C}$  which will increase the overall efficiency of the process. For the electrolysis of  $\text{SO}_2$  at high temperature, MEAs including PBI-Based membranes are proposed. Thus, the challenge does not only regard membrane stability but also, catalyst durability and operation parameters. In this work, the chemical resistance of different PBI membranes and  $\text{H}_3\text{PO}_4$  and  $\text{H}_2\text{SO}_4$  as doping agents were studied for the  $\text{SO}_2$  electro-oxidation.

### Acknowledgements

Financial support from the Junta de Comunidades de Castilla-La Mancha and FEDER -EU Program, Project ASEPHAM. Grant number "SBPLY/17/180501/000330" is gratefully acknowledged.

### Biography: Sergio Díaz Abad

Sergio Díaz is a PhD student at the Department of Chemical Engineering, University of Castilla-La Mancha of Spain. He received his BSc in chemical engineering and his Master's in Chemical Engineering from the same university. He also gained experience in research in an intership at EMPA Swiss Federal Laboratories, Switzerland, between 2017 and 2018. The focus of his current research is the development of advance materials for the sulfur dioxide depolarized electrolysis.

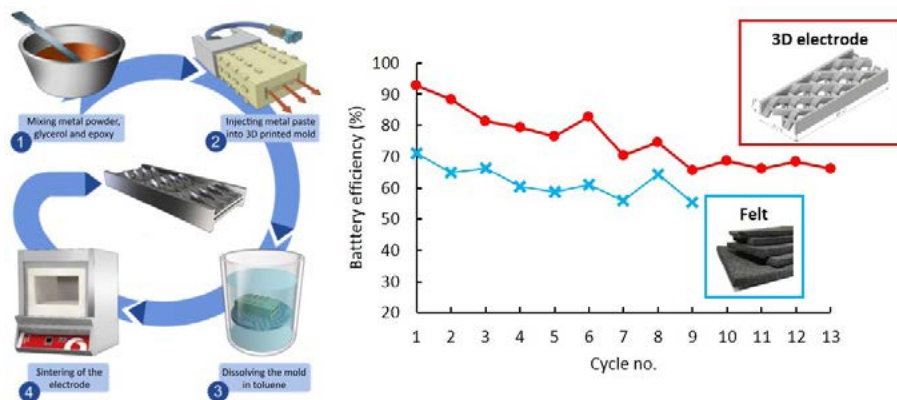
### 255 | Improving the hydrodynamics of redox flow batteries through 3D printed electrodes

Jonas Hereijgers (University of Antwerp, Research Group Applied Electrochemistry & Catalysis (ELCAT)), Renée De Wolf (University of Antwerp, Research Group Applied Electrochemistry & Catalysis (ELCAT)), Tom Breugelmans (University of Antwerp, Research Group Applied Electrochemistry & Catalysis (ELCAT))

#### Abstract

Redox flow batteries are an interesting technology to store electricity of renewable intermittent power sources such as wind mills and solar panels. In redox flow batteries, the electrolyte is pumped actively through the electrochemical cell, resulting in a storage capacity that is no longer dependent on the size of the battery pack as is the case with conventional Li-ion batteries. To maximize the power output of redox flow batteries, they are typically equipped with 3D electrodes such as felt and carbon paper electrodes to enlarge the electrode area. However, such disordered electrode geometries result in non-uniform flow distributions, negatively affecting the reagent turnover rate and pressure loss, reducing the overall system efficiency accordingly.

In this work we present structured 3D printed electrodes that show unprecedented hydrodynamic and mass transport properties. Through its ordered geometry, the pressure loss with these 3D electrodes was two orders of magnitude lower than a commercial felt electrode. As a result the pumping power to circulate the electrolyte decreased from 213 mW/kg to 0.75 mW/kg. In this way mass transfer limitation in a redox flow battery was improved, resulting in a 10 to 20% higher efficiency, surpassing the current state-of-the-art felt electrodes.



#### Biography: Jonas Hereijgers

Dr. Ing. J. Hereijgers finished his PhD at the University of Brussels in 2016 and is since then a postdoctoral researcher at the University of Antwerp in the field of electrochemical engineering. Currently, he is author of 29 A1 publications and works on improving the hydrodynamic and mass transfer properties in electrochemical reactors. In collaboration with Prof. M. Wessling (RWTH Aachen University) he developed 3D printed electrodes for electrochemistry such as redox flow batteries, improving hydrodynamic and mass transfer properties in electrochemical reactors with over two orders of magnitude.

### 362 | Development of electrochemical processes to reduce environmental risk of Hospital Effluents

Engracia Lacasa (University of Castilla-La Mancha), Cristina Sáez (University of Castilla-La Mancha), Angela Moratalla (Department of Chemical Engineering, University of Castilla-La Mancha), Salvador Cotillas (University of Castilla-La Mancha), Pablo Cañizares (University of Castilla), Manuel A. Rodrigo (University of Castilla-La Mancha)

#### Abstract

In last decade, reducing environmental threat of pharmaceuticals has become a priority, and treatment of hospital wastewater has been the target of many researches, using biological and chemical oxidation treatments, membrane processes or Advanced Oxidation Processes [1]. Among them, Electrochemical Advanced Oxidation Processes (EAOPs) seem to be a good alternative to reduce the risk of hospital effluents but more scientific effort is needed for large-scale application, mainly in the aspect of reducing the formation of un-desirable by-products and the ecotoxicity risk, as well as improving energy efficiency and reducing operational cost. Therefore, the goal of this work is the design of an electrochemical reactor to reduce hazardousness of hospital effluents. This is a complex process in which many aspects must be considered: electrode material, electrode configuration, flow dynamic conditions and, obviously, operating conditions.

#### References

[1] Soliu O. Ganiyu, Eric D. van Hullebusch, Marc Cretin, Giovanni Esposito, Mehmet A. Oturan, Separation and Purification Technology, Volume 156, Part 3, 2015, Pages 891-914.

#### Acknowledgements

This work is supported by Junta de Comunidades de Castilla-La Mancha and Ministry of Science and Innovation through the projects SBPLY/17/180501/000396 and PID2019- 110904RB-I00 through “Juan de la Cierva” grant (JC2018-036241-I) awarded to Dr. Salvador Cotillas.

## 226 | Theoretical and experimental characterization of $H_2O/H_2$ flow in an electrocoagulation reactor in serpentine array

*Locksley Castañeda (Universidad de Guanajuato), José L. Nava (Universidad de Guanajuato)*

### Abstract

During the electrocoagulation (EC) processes, large amounts of hydrogen bubbles are generated at the cathode from the reduction of water, while the coagulant, aluminum or iron complexes, are formed during the dissolution of the sacrificial anode. The  $H_2$  formation, dispersed phase, provokes dispersion of the continuous phase flow,  $H_2O$ , in flow cells used as EC reactors. Moreover,  $H_2$  bubbles also impacts the current distribution on the electrodes, affecting the current efficiency, the electrolytic energy consumption and the performance of the cells. This work deals with the two-phase ( $H_2O-H_2$ ) flow characterization in a continuous EC reactor with a six-cell stack in serpentine array.

The  $H_2O-H_2$  flow was simulated using the Euler- Euler approach, solving the Navier-Stokes (NS) equations through the finite element method. In order to perform a more complete flow pattern characterization, residence time distribution (RTD) studies were performed to validate the CFD simulations. Theoretical RTD curves were calculated solving the averaged diffusion-convection equation. Close agreement between experimental and theoretical RTD curves were obtained. On the other hand, the Bruggeman relation was used to compute the current density distribution on the electrodes in the stack, observing changes of 10% in the current distribution attributed to the  $H_2$  formation on the cathodes.

### Biography: Locksley Castañeda

LOCKSLEY F. CASTAÑEDA is a professor associated to University of Guanajuato. He received his bachelor's degree in chemical engineering from the Technological Institute of Tepic and both his MSc and PhD degrees in Electrochemistry were obtained from the Center for Research and Technological Development in Electrochemistry (CIDETEQ), besides, he has a postdoctoral degree from the University of Guanajuato. His main research interests include the design and simulation of electrochemical reactors through computational fluid dynamics, wastewater treatment through electrochemical processes, as electro dialysis, electroperoxone, electrocoagulation, among others.

## 150 | Effect of operating conditions on performance and lifetime of vanadium-oxygen fuel cell

*Jiří Charvát (University of Chemistry and Technology, Prague), Petr Mazúr (University of Chemistry and Technology, Prague), Jindřich Mrlik (University of Chemistry and Technology, Prague), Jan Dundálek (University of Chemistry and Technology, Prague), Juraj Kosek (University of Chemistry and Technology, Prague), Martin Paidar (University of Chemistry and Technology, Prague), Jaromír Poceďič (University of West Bohemia)*

### Abstract

Vanadium redox flow battery is one of the most developed type of stationary energy storage technology but it has some disadvantages such as low energy density and relatively high price. A vanadium oxygen fuel cell, where the positive electrolyte ( $VO_2+/VO_2+$  couple) is replaced by oxygen reduction, could significantly improve energy density and reduce costs of capacity as only negative electrolyte is used. Moreover, concentration of vanadium electrolyte can be substantially increased when compared to standard vanadium redox flow battery where positive electrolyte is the limiting one.

In this work performance of lab-scale vanadium oxygen fuel cell is studied for different internal components (gas diffusion electrode, ionexchange membrane) and arrangements of the cell. The efficiency and performance stability under various operational conditions (current load, air flow rate and humidity, temperature) was determined from constant current discharging at 50 % state of charge (external electrolyser was used to maintain constant state of charge). Internal resistance of the cell was determined from electrochemical impedance spectra and load curves. Based on the results the main sources of the cell inefficiency are identified and strategies towards improved efficiency are suggested and tested.

### Biography: Jiří Charvát

I am a PhD student at Department of Chemical Engineering at University of Chemistry and Technology in Prague. During my bachelor and master studies my research was related to vanadium redox flow batteries, specifically to ionexchange membranes and carbon felt electrodes and last year I have started with research of vanadium-oxygen fuel cell as part of my dissertation.

## 260 | Electrochemical oxidation of ammonia coupled with hydrogen generation

John Graves (Coventry University), Liang Wu (Coventry University), Egle Latvyte (Coventry University), Peter Vale (Severn Trent Water Ltd.)

### Abstract

Interest in using hydrogen as a fuel is gaining momentum. This is primarily driven by the need to cut energy related CO<sub>2</sub> emissions. Today, 95% of hydrogen produced globally is derived from non-renewables. A goal of the hydrogen economy is to develop affordable methods for producing hydrogen which are not reliant upon fossil fuels. Ammonia is a carbon-free chemical energy carrier. The theoretical potential for ammonia oxidation (0.06V) is much lower than that for water oxidation (1.23V). A low cell voltage has the potential to lead to a reduction in electrolyser operating costs. Ammonia is a pollutant, present in municipal wastewater streams. Current ammonia treatment processes consume large amounts of energy and have high operational costs. Ammonia electro-oxidation can be combined with hydrogen generation at the cathode. Ammonia remediation coupled with hydrogen production, has greater value than using ammonia as a fertiliser. Consequently, the focus of this research is to develop an efficient, low cost, ammonia electrolyser which couples the destruction of ammonia with the generation of hydrogen. Success will lead to new opportunities for wastewater treatment companies and the possible use of ammonia as an energy vector, see Figure 1.

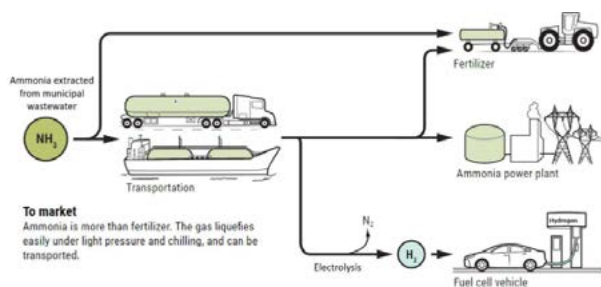


Figure 1. Adapted from V. Altounian/Science, Possible uses of ammonia (Source: <https://www.sciencemag.org/news/2018/07/ammonia-renewable-fuel-made-sun-air-and-water-could-power-globe-without-carbon>)

### Biography: John Graves

Dr. John Graves is an Associate Professor in the Institute for Future Transport and Cities Research Centre at Coventry University and has a passion for the generation of hydrogen from non-fossil fuel sources to support the hydrogen economy. He received his Ph.D. in Electrochemistry from Southampton University and joined a specialty chemicals company where he became the European Research Manager for metallization products. He has been an assessor for the European Commission and the British Council and is a longstanding Fellow of the Royal Society of Chemistry.

## Plenary: Complexants as active modulators of metal surface reactivity: from Corrosion Control to Primary Batteries

Mikhail Zheludkevich

Institute of Surface Science, Helmholtz-Zentrum Geesthacht,  
Max-Planck Str. 1, 21502 Geesthacht, Germany

Magnesium and its alloys are among the lightest structural metallic materials and also considered as promising materials for resorbable implants and energy storage. However, the high reactivity and the corrosion susceptibility of Mg in aqueous environments significantly limits the application range. However, the reactivity of the Mg surface can be controlled from both the metal and the electrolyte sides.

In this paper, the chelating agents able to form complexes with Mg cations and the cations of impurity elements are discussed as potential modulators of Mg surface reactivity.

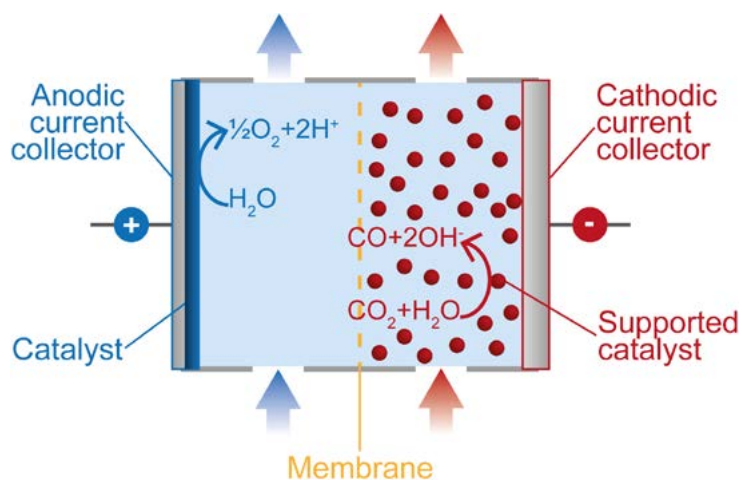
The compounds capable to form strong insoluble complexes with Mg<sup>2+</sup> can confer an efficient inhibition of Mg dissolution blocking the surface by a dense layer of products. In turn, the modulators forming highly soluble complex can strongly affect formation of the corrosion products on the metal surface shifting the process towards faster dissolution of Mg, which can be relevant for the optimization of discharge properties of metallic Mg-based anodes. The talk will also address the strategies for selecting efficient modulators with targeted properties using Artificial Intelligence based approaches.

### 601 | Suspension electrodes for enhanced mass transfer in electrocatalytic CO<sub>2</sub> reduction

Nathalie Ligthart (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands), Laura Donk (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands), David Vermaas (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands)

#### Abstract

When intensifying electrochemical energy conversion processes that deal with low-concentrated reactants (like resource recovery or CO<sub>2</sub> conversion), mass transport limitations occur and cause low Faradaic efficiencies (FE) at high current densities. We investigate whether mass transport can be improved by using flowable suspension electrodes instead of stationary electrodes. In case of CO<sub>2</sub> reduction to CO, H<sub>2</sub> evolves as a side product because of slow CO<sub>2</sub> transfer. In this study, we assess the performance of suspension electrodes for CO<sub>2</sub> reduction by comparing the achieved FEs at high current densities with a similar flow cell using a stationary electrode. We synthesize and use suspensions of activated carbon powder coated with silver nanoparticles as electrocatalyst in CO<sub>2</sub>-saturated 0.5 M aqueous KHCO<sub>3</sub> solution, and tested this flowable cathode in an electrochemical flow cell, with a stationary Ir-oxide coated anode. This system opens up a route to enhanced mass transfer in electrochemical energy conversion processes.



#### Biography: Nathalie Ligthart

Nathalie Ligthart is a Ph.D. candidate in the Transport Phenomena group within the Faculty of Applied Sciences at Delft University of Technology, The Netherlands. She is working on suspension electrodes for enhanced mass transport in electrochemical flow systems, under supervision by David Vermaas. Before joining the TU Delft, she received her MSc degree in Nanomaterials Science and her BSc degree in Chemistry from Utrecht University in the Netherlands.

### 605 | Optimization study of acid-base flow battery stacks with monopolar and bipolar membranes

Andrea Culcasi, Luigi Gurreri, Alessandro Tamburini, Giorgio Micale (University of Palermo, Italy)

#### Abstract

The Acid-Base Flow Battery (AB-FB) is a novel technology for energy storage. It is based on reversible electrochemical techniques with ionexchange membranes. The key elements are the bipolar membranes, which convert electrical energy in the form of pH gradients and vice versa. Despite the promising results of few experimental studies, the AB-FB potential has been poorly explored so far.

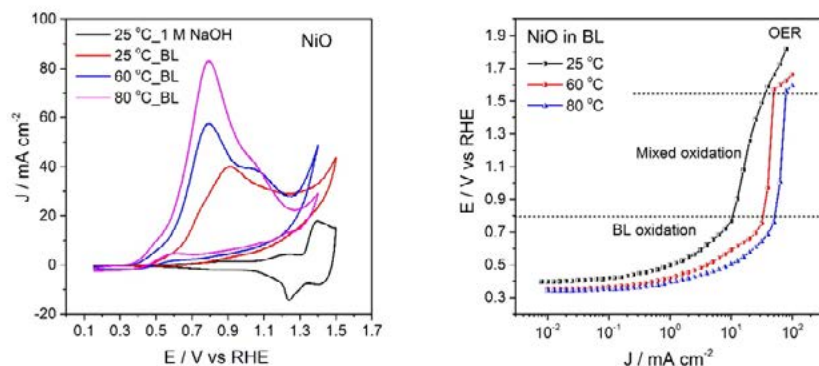
This work presents an optimization study of the AB-FB. It was performed by a multi-process model previously developed (gPROMS Model Builder® environment) and experimentally validated. A two-objective optimization was conducted by maximizing the Net Round Trip Efficiency and the Net Power Density in the discharge phase. By the  $\epsilon$ -constraint method, curves of Pareto optimal solutions were predicted under several scenarios by assessing systematically the effect of decision variables. In a closed-loop configuration (solutions recirculation), optimized operating conditions and design features yielded a maximum NRTE of 64% and a maximum NPD of 19.5 Wm<sup>-2</sup>. Improved membrane properties increased these quantities to 76.2% and 23.2 Wm<sup>-2</sup>, respectively. Finally, open-loop operations were beneficial for the process performance. These promising results will drive the AB-FB technology towards future developments and competitive configurations.

## 610 | Promising Hydrogen Production from Black Liquor Electrolysis on Earth-Abundant Catalysts

Zhen Qiu (Division of Applied Electrochemistry, Department of Chemical Engineering, KTH Royal Institute of Technology, SE-10044, Stockholm), Pär Lindén (Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-10044, Stockholm), Gunnar Henriksson (Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-10044, Stockholm), Ann Cornell (Division of Applied Electrochemistry, Department of Chemical Engineering, KTH Royal Institute of Technology, SE-10044, Stockholm)

### Abstract

Hydrogen is considered as a promising energy carrier to address sustainability, environmental emissions, and energy security issues. Here, we present a hydrogen production pathway combined with the electrolysis of black liquor. This study focuses on the anodic oxidation of birch black liquor for energy conversion. NiPd and NiO have been investigated as an anode material for birch black liquor oxidation at a range of temperatures and current densities. From polarization curves we found that the active potential window of black liquor on catalysts was less than 0.8 V vs RHE, well shifted from the oxygen evolution reaction. Notably, the earth-abundant electrocatalyst NiO exhibited excellent performance for birch black liquor oxidation, only requiring 0.57 V vs RHE to reach 10 mA cm<sup>-2</sup> with a Tafel slope of 23.9 mV dec<sup>-1</sup> at 80 °C. It provides a dramatic decrease in energy requirement compared with conventional water electrolysis. The cost-efficiency suggests that NiO is a promising electrode material for the application of black liquor electrolyzers. This work shows the potential to boost the energy efficiency of the Kraft pulp process.



(Left) Potential sweeps at a scan rate of 10 mV s<sup>-1</sup> and (Right) polarization curves on NiO for birch black liquor oxidation.

### Biography: Zhen Qiu

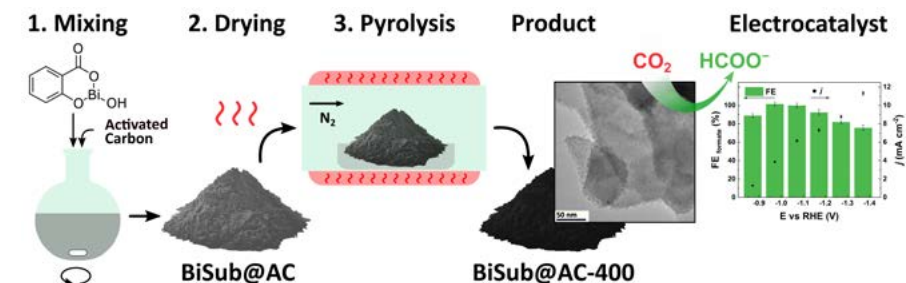
DR. ZHEN QIU is currently a Postdoc at KTH Royal Institute of Technology at the Division of Applied Electrochemistry in the electrolysis group of Prof. Ann Cornell. She completed her Ph.D. in 2019 at Uppsala University (Sweden), mainly working on the transition metal-based electrocatalysts for alkaline water splitting and CO<sub>2</sub> reduction. Her current research focuses on the scale-up of hydrogen production by electrolysis of biomass, mainly on Kraft black liquor.

## 537 | Scalable Bismuth electrocatalyst for selective CO<sub>2</sub>-to-formate conversion

Matteo Miola (Sustainable Chemical Products and Catalysis Chemical Engineering Group, ENTEG, University of Groningen), Bart C. A. De Jong (Sustainable Chemical Products and Catalysis Chemical Engineering Group, ENTEG, University of Groningen), Paolo Pescarmona (Sustainable Chemical Products and Catalysis Chemical Engineering Group, ENTEG, University of Groningen)

### Abstract

The electrochemical conversion of CO<sub>2</sub> to valuable products is a particularly appealing technology for the mitigation of anthropogenic CO<sub>2</sub> emissions. Among the obtainable CO<sub>2</sub> electrochemical conversion products, formate is a relevant target, owing its high accessibility (2 e<sup>-</sup> process) and its broad range of applications. [1] Here, we present a novel, straightforward and scalable synthesis procedure of a highly selective electrocatalyst for conversion of CO<sub>2</sub> to HCOOH. The synthesis involves the impregnation of a lowcost and abundant organic bismuth precursor (bismuth subsalicylate, BiSub) on activated carbon, followed by low temperature pyrolysis (T= 400°C). The obtained BiSub@AC-400 material consists of small and highly dispersed Bi NPs (Ø~ 6 nm – see TEM below) supported on activated carbon (AC). The electrocatalyst shows complete selectivity (FE > 99%) at E = -1.07 V vs RHE in CO<sub>2</sub>-saturated 0.5 M NaHCO<sub>3</sub> electrolyte (see figure below) and high stability, maintaining a current density of ~4 mA cm<sup>-2</sup> at E = -0.97 V vs RHE for 48 h. [1] We are currently studying and will report the electrocatalyst behaviour under industrial relevant flow conditions (j<sub>CO<sub>2</sub></sub> > 100 mA cm<sup>-2</sup>).



### Biography: Matteo Miola

Miola et al. CHEM. COMMUN., 2020,56, 14992-14995 (<https://doi.org/10.1039/D0CC06818G>)

### 533 | Stable Organic Radicals for Symmetric Redox Flow Batteries

Jelte Steen (Stratingh Institute for Chemistry, University of Groningen), Edwin Otten (Stratingh Institute for Chemistry, University of Groningen), Jules Nuismer (Stratingh Institute for Chemistry, University of Groningen), Vytautas Eiva (Stratingh Institute for Chemistry, University of Groningen), Johan Hjelm (DTU ENERGY, Technical University of Denmark)

#### Abstract

Energy production from fossil fuels is steadily replaced by green, renewable alternatives such as solar and wind power. Due to the intermittent energy production from these sources, incorporation of large-scale energy storage has been identified to be critical for ensuring a stable future energy supply. Redox Flow Batteries (RFBs) have gained increased attention as cheap and scalable storage solution due to their decoupling of power and energy and simplicity of design.

The price volatility and environmental concerns associated with classical vanadium-based RFBs has led to the development of alternative battery chemistries. RFBs that use organic compounds as charge-storage material hold considerable promise, but these often suffer from capacity fade due to crossover of redox active material. One approach to circumvent this issue is to use a symmetric RFB, consisting of one bipolar molecule that can be both reversibly reduced and oxidized to facilitate both electrode half-reactions.

In this presentation, we present a study on the performance of two highly promising classes of nitrogen-rich organic radicals as bipolar charge storage material for both non-aqueous and aqueous symmetric RFB applications.

#### Biography: Jelte Steen

Jelte Steen was born in 1994 and raised in Marrum, a village near Leeuwarden. In 2014, he received his BSc degree working in the group of Prof. Dr. Gerard Roelfes on cell-targeting drugs. Hereafter, he joined the Otten group to work on his masterproject about cyclic formazanate metal complexes. Subsequently, he performed a short internship under the supervision of prof. Xavi Ribas at the IQCC in Girona, working on supramolecular metallocages. Hereafter, he returned to Groningen and the Otten group to pursue a PhD. Currently, he is working on the synthesis and application of organic radicals for symmetric RFBs.

### 196 | Proton and oxygen management in electrocatalysis on conducting polymers

Mikhail Vagin (Laboratory of Organic Electronics, ITN, Linköping University)

#### Abstract

The electrocatalytic processes for the energy conversion are the key aspects in the development of sustainable economy. Being one of the main technological stimuli of electrocatalysis research, the direct chemical-to-electrical energy interconversion is employed in a variety of applications from the electrical transportation to the balancing of the grid. Among the examples of the electrocatalytic processes, where the wide commercialization is limited by the cost of catalysts, the oxygen reduction reaction (ORR) and the hydrogen evolution reaction (HER) are the most critical for the development of technological infrastructure of fuel cells. This stipulates the intensive research on noble-metal-free electrocatalysts. The quantification of ORR and HER on the intrinsically conducting polymers allows the rational design of catalyst, systematic investigation of mass transport phenomena and mechanistic evaluation of electrocatalysis due to the open material architecture. Firstly, the landscape of ORR phenomena happening on conjugated polymers is discussed at the mechanistic and device levels. The effects of cocatalyst and proton supply on ORR efficiency and the pathway is illustrated on the examples of poly(3,4-ethylenedioxythiophene) (PEDOT) as organic ORR catalyst [DOI: 10.1039/c6ta10521a, 10.1002/adsu.201800110, 10.1002/adsu.2019000971-3]. Secondly, the effect of proton supply is rationalized at both mechanistic and device levels for HER on PEDOTtriflate [DOI: 10.1039/c9se00687g].

#### Biography: Mikhail Vagin

Dr. M. Vagin started his research career in field of applied electrochemistry in 1997 at Chemistry Faculty of M.V. Lomonosov Moscow State University as an undergraduate student (start 1997; 1998 MSci; 2002 PhD) and ended in 2010 as a full-time senior researcher. Then he worked as a postdoctoral researcher in two research institutes in Ireland. He joined Linköping University as a postdoctoral researcher in 2012. He became a docent in physical chemistry in 2019. The main scientific interests are focused on the mechanism- and the device-oriented aspects of electrocatalysis.

### 330 | Role of Different Electrolytes in CO<sub>2</sub>RR – Improvements in FE and Product Selectivity

Marlia Pupo (TU Delft), Ruud Kortlever (TU Delft)

#### Abstract

The electrochemical reduction of CO<sub>2</sub> to valuable products can serve to utilize CO<sub>2</sub> as a feedstock for the production of bulk chemicals for industry, and as a means to store renewable energy in chemical bonds. Low product selectivities and relatively high overpotentials are limiting the industrial implementation of the process [1-3]. However, pH regulation and proton availability are found to be important factors affecting the products distribution and Faradaic efficiency. Therefore, electrolyte engineering can play a key role in devising more selective and efficient electrochemical CO<sub>2</sub> reduction processes.

The presented study carries out a thorough investigation on the role of different electrolytes in the tailoring the product selectivity of the CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR). Using a lab-scale flow-cell, we analyze the Faradaic efficiency toward different products when employing different non-aqueous electrolyte mixtures. Mixtures of acetonitrile, ionic liquid, and water, with varying concentrations, were used as electrolytes and product formation was analyzed through GC and HPLC. From the data obtained, it is possible to observe how the product distribution and selectivity is affected by proton availability, pH, and presence of anions in the solution leading to a rapid and facile route to control and alter the final products obtained from CO<sub>2</sub>RR.

#### Biography: Marilia Pupo

PostDoc at TU Delft working on electrochemical CO<sub>2</sub> reduction optimization through analysis of electrolyte influence.

### 448 | Lab-scale experiments on a novel acid/base electrolysytic flow battery with bipolar membranes

Luigi Gurreri (University of Palermo), Alessandro Cosenza (University of Palermo), Andrea Zaffora (University of Palermo), Luca Muratore (University of Palermo), Domenico Antonino Agnello (University of Palermo), Alessandro Tamburini (University of Palermo), Giorgio Micale (University of Palermo)

#### Abstract

Electrical energy storage has a key role in the development and diffusion of renewable energy technologies. The Acid/Base Flow Battery is an innovative process to store electrical energy in the form of pH and salinity gradients via electrolysytic reversible techniques based on the use of bipolar membranes. During the charge phase, the unit produces acid and alkaline solutions by applying an electric field, during the discharge phase, converts the pH gradient into electrical energy.

In this work, several experimental tests were performed in a 10×10 cm<sup>2</sup> laboratory-scale unit fed with HCl, NaOH and NaCl solutions, in order to characterize the battery and assess its performance. The effect of acid/base concentration, feed velocity and the number of repetitive units (triplets) was studied. Results showed that the Open Circuit Voltage obtainable with 1 M acid/base solutions increases from 4.2 V in a stack equipped with 5 triplets to only 16.5 V in a stack equipped with 38 triplets, due to significant effects of shunt currents, with a maximum power density of about 18 W/m<sup>2</sup> in the discharge phase. Other important limitations originate from co-ion leakages. This work was performed in the framework of the BAoBaB project, funded by the EU H2020 program.

#### Biography: Luigi Gurreri

PhD in Chemical Engineering. Post-doc with research activity on CFD and mathematical modelling of membrane processes for desalination, salinity gradient energy, and pH gradient flow batteries.



### 93 | NiCoP cathode catalyst for electrochemical water splitting: Structural and electrochemical characterization

Martin Durovic, Jaromír Hnát, Karel Bouzek (University of Chemistry and Technology, Prague, Dep. of Inorganic Technology)

#### Abstract

Alkaline water electrolysis is an industrial process that could convert excess electrical energy from renewable energy sources (RES) into hydrogen. However, since this technology was designed for long-term stable operation, the combination with RES places new demands on the process. One of the important topics how to increase its flexibility and efficiency is to find an active, inexpensive and stable electrocatalyst for hydrogen evolution reaction (HER).

In this work, NiCoP catalyst was synthesized by cathodic electrodeposition on Ni substrate in a deposition bath ( $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ ,  $\text{NaH}_2\text{PO}_2 \cdot \text{H}_2\text{O}$ ). The effect of (i) the deposition solution composition and (ii) the current density (-100, -75, -50, -25 mA cm<sup>-2</sup>) on the catalyst activity, composition and morphology was determined by several analytical and electrochemical methods, such as TEM, SEM-EDS, Tafel analysis, cyclic voltammetry, electrochemical impedance spectroscopy etc. The structural characterization showed that multiple phases are formed during the electrodeposition. The catalyst composition is not dependent on the current density but can be adjusted by the deposition solution composition. The electrochemical studies suggest excellent catalytic activity for HER in an alkaline environment.

Financial support by the Technology agency of the Czech Republic (TK02030103) and specific university research (MSMT No 21-SVV/2020) is gratefully acknowledged.

#### Biography: Martin Durovic

The author is a Ph.D. student at the University of Chemistry and Technology in Prague. He graduated from the study program: Hydrogen and Membrane Technologies (diploma thesis: Optimization of the cathodes catalytic layer for alkaline water electrolysis). His main research is focused on the electrocatalysts for alkaline water electrolysis and fuel cells. The author also successfully published an article entitled "Nanocrystalline  $\text{Fe}_{60}\text{Co}_{20}\text{Si}_{10}\text{B}_{10}$  as a cathode catalyst for alkaline water electrolysis: Impact of surface activation" in an impacted journal *Electrochimica Acta*.

### 79 | Real-time characterization of CO<sub>2</sub> reduction products

Mario Löffler (Forschungszentrum Juelich GmbH), Peyman Khanipour (Forschungszentrum Juelich GmbH), Andreas M. Reichert (Forschungszentrum Juelich GmbH), Ioannis Katsounaros (Forschungszentrum Juelich GmbH)

#### Abstract

The classical way to characterize reaction products in electrochemistry involves steady-state electrolysis combined with intermittent product determination, for example with chromatography, nuclear magnetic resonance etc. While these methods enable quantification in terms of faradaic efficiencies and reaction rates, they offer temporal resolution in the order of several minutes. Therefore, it is not possible to determine the product formation under dynamic conditions.

We recently developed an internationally unique method to characterize the products of electrochemical reactions at the time they are formed, the \_electrochemical real-time mass spectrometry\_ (EC-RTMS). Contrary to previous approaches, EC-RTMS is not limited by the vapor pressure of analytes or the presence of nonvolatile salts. The basic principles of EC-RTMS will be presented, together with the real-time characterization of products of the CO<sub>2</sub> reduction reaction on copper-based electrodes.

#### Biography: Ioannis Katsounaros

- 2005-2009: PHD, Aristotle University of Thessaloniki, Greece
- 2010-2013: POST-DOC, Max Planck Institute Düsseldorf, Germany
- 2013-2016: MARIE CURIE INTERNATIONAL OUTGOING FELLOW at the Argonne National Lab, USA (2-year outgoing phase) and the University of Leiden, The Netherlands (1-year return phase)
- 2016-NOW: GROUP LEADER at the Helmholtz Institute Erlangen-Nuremberg, an institute of the Research Center Jülich, Germany.

## 71 | Metal phosphides as cathodes in PEM water electrolysis

*Foteini Sapountzi (Syngaschem BV), Georgios Zafeiropoulos (Dutch Institute For Fundamental Energy Research), Yury V. Kolen'ko (International Iberian Nanotechnology Laboratory), Juliana P.S. Sousa (International Iberian Nanotechnology Laboratory), Kirill Kovnir (Iowa State University), Bryan Owens-Baird (Iowa State University), J.W. (Hans) Niemantsverdriet (Syngaschem BV)*

### Abstract

Water electrolysis allows conversion of surplus renewable electricity to chemical energy, by producing hydrogen for end-use and as an energy storage medium. Alkaline water electrolysis relies on abundant electrocatalysts, but its market penetration is still low due to limited efficiency and insufficient compatibility with the intermittency of renewables. On the other hand, proton exchange membrane (PEM) electrolyzers utilize a polymer electrolyte instead of an aqueous one. This zero-gap design offers high currents and responsiveness to variable power input. However, the commercialization of PEM electrolysis has been hindered by the requirements of platinumgroup metal electrocatalysts, which can withstand the acidic nature of the proton exchange membrane. To address this issue, research in the field has been directed towards the development of acid-stable low-cost electrocatalysts. Our work focuses on the applicability of such emerging materials into realistic systems as a next step for assessing the viability of these technologies. Using transition metal phosphides as the showcase, suitable engineered membrane-electrode assemblies have been developed and tested in single-cell devices under realistic conditions. We will present two examples of metal phosphides used as cathodes in PEM water electrolysis, which show appreciable activity (13% higher overpotentials than Pt) and stability for several days of testing.

### Biography: Foteini Sapountzi

Foteini Sapountzi obtained her PhD in Chemical Engineering in 2009 from the University of Patras (Greece), supervised by Prof. Vayenas. She continued working at the same group till 2011, when she joined the group of Prof. Valverde at University of Castilla La Mancha (Spain). From 2012 till 2014 she worked with Dr. Vernoux at IRCELYON/CNRS (France). Since 2015, Foteini works as a Research Scientist at Syngaschem BV (Netherlands) collaborating with by Prof. Niemantsverdriet. Her activities are focused on the electrochemical engineering of zero-gap water electrolyzers. She has co-authored 28 articles, including a comprehensive review on water electrolysis technologies.

## 683 | Advances and challenges in understanding the electrocatalytic conversion of carbon dioxide to fuels

*Marc T.M. Koper (Leiden Institute of Chemistry, Leiden University)*

### Abstract

The electrocatalytic reduction of carbon dioxide is a promising approach for storing (excess) renewable electricity as chemical energy in fuels. Here, I will discuss recent advances and challenges in the understanding of electrochemical CO<sub>2</sub> reduction. I will summarize existing models for the initial activation of CO<sub>2</sub> on the electrocatalyst and their importance for understanding selectivity. Carbon-carbon bond formation is also a key mechanistic step in CO<sub>2</sub> electroreduction to high-density and high-value fuels. I will show that both the initial CO<sub>2</sub> activation and C-C bond formation are influenced by an intricate interplay between surface structure (both on the nano- and on the mesoscale), electrolyte effects (pH, buffer strength, ion effects) and mass transport conditions. This complex interplay is currently still far from being completely understood.

Y.Y.Birdja, E.Perez-Gallent, M.C.Figueiredo, A.J.Göttle, F.Calle-Vallejo, M.T.M.Koper, *Nature Energy* 4 (2019) 732-745

### References

1. Surname, M. *Angew. Chem., Int. Ed. Engl.* 1989, 28, 322-325.
2. Surname, R. *J. Bioorg. Med. Chem.* 2002, 10, 3379-3383.

## 197 | Charging Mechanisms and Dynamics in Supercapacitors from NMR Spectroscopy

Alexander Forse (University of Cambridge)

### Abstract

Supercapacitors are high power energy storage devices that can complement batteries in a more sustainable future. A detailed understanding of the mechanisms of charge storage in these devices is key to their optimisation. We have developed NMR spectroscopy as a powerful experimental probe of the interface between porous carbons and electrolytes.<sup>1</sup> NMR allows charge-storing ions in the electric double-layer to be distinguished from those in bulk electrolyte. *In situ* NMR measurements on working devices allow the ionic composition of the carbon pores to be measured at different cell voltages. We show that a number of different charge storage mechanisms can operate, depending on the chosen electrolyte and the polarisation of the electrode.<sup>2</sup> We also show how pulsed field gradient NMR can be used to track the diffusion of ions in the electric double-layer of working supercapacitors, and how this can explain their charging rates.<sup>3</sup> Our experiments give a , and can facilitate the development of new devices with improved performances.

### References

<sup>(1)</sup> Forse, A. C.; et al. *J. Am. Chem. Soc.* 2016, *138*, 5731–5744.

<sup>(2)</sup> Griffin, J. M.; et al. *Nat. Mater.* 2015, *14*, 812–819.

<sup>(3)</sup> Forse, A. C.; et al. *Nat. Energy* 2017, *2*.

### Biography: Alexander Forse

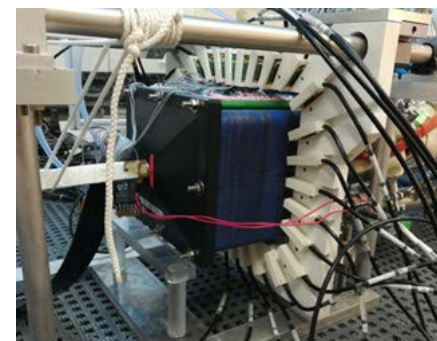
Dr Alexander Forse is a Lecturer in Materials Chemistry in at the University of Cambridge. The Forse Group seeks to understand and improve materials that can reduce greenhouse gas emissions and tackle the global warming crisis. Focus areas include energy storage, carbon dioxide capture, and electrochemical separations.

## 425 | Fault detection and identification for Polymer Electrolyte Membrane Fuel Cell

Yann Bultel (Univ. Grenoble Alpes, Univ. Savoie-Mont Blanc, CNRS, Grenoble INP, LEPMI, 38000 Grenoble, France), Helen Barboza-da-silva (Univ. Grenoble Alpes, CNRS, Grenoble INP, G2Elab, F-38000 Grenoble, France), Salah Touhami (Univ. Lorraine, CNRS, LEMTA, 54500 Vandoeuvre-lès-Nancy, France), Gilles Cauffet (Univ. Grenoble Alpes, CNRS, Grenoble INP, G2Elab, F-38000 Grenoble, France), Olivier Chadebec (Univ. Grenoble Alpes, CNRS, Grenoble INP, G2Elab, F-38000 Grenoble, France), Olivier Lottin (Univ. Lorraine, CNRS, LEMTA, 54500 Vandoeuvre-lès-Nancy, France), Sébastien Rosini (Univ. Grenoble Alpes, CEA, LITEN, F-38054 Grenoble, France)

### Abstract

Reliability and durability are key considerations to successfully deploy Proton Exchange Membrane Fuel Cells (PEMFCs). So, effective tools are required to control their mass-production, the quality of the stacks and their diagnosis for onsite maintenance (stationary) or for on-board (transportation) applications. Therefore, techniques sensitive to localized phenomena are of major interest in the development of PEMFC diagnosis. In perspective, local electrochemical measurement associating current density distribution and local Electrochemical Impedance Spectroscopy (EIS) may support stack-level degradation analyses as well as effective control to mitigate the consequences of degradation due to load cycles (electrochemical, thermal, mechanical and humidity effects) or faults. The key here is to extract information about local current density distribution and impedance, over either a cell or a stack. This strategy requires the complementary development of segmented cells as well as magnetic field techniques, to implement local measurement respectively over MEA surface and onto stack during real-life operation. This challenge is tackled by using tailored defective MEAs or thanks to specific operating conditions (flooding, drying, ...) to characterize how local and overall performances of the MEA are affected and to identify the signatures of the various anomalies.



### Biography: Yann Bultel

YANN BULTELE is Professor at Grenoble-INP. He has a 23-year experience in electrochemical engineering, especially regarding the characterisation and modeling of Fuel Cells and Batteries. He authored 103 publications in peerreviewed journals, 2 book chapters, 1 patent and gave more than 200 communications in (inter)national conference. He led the Hychain project (2006-2011) and 8 ANR projects for Grenoble INP. He supervised more than 20 PhD theses since 2000.

### 288 | Engineering an industrial CO<sub>2</sub> electrolyzer

Tom Breugelmans (University of Antwerp, Research Group Applied Electrochemistry & Catalysis (ELCAT)), Bert De Mot (University of Antwerp, Research Group Applied Electrochemistry & Catalysis (ELCAT)), Miguel Duarte (University of Antwerp, Research Group Applied Electrochemistry & Catalysis (ELCAT)), Nick Daems (University of Antwerp, Research Group Applied Electrochemistry & Catalysis (ELCAT)), Jonas Hereijgers (University of Antwerp, Research group Applied Electrochemistry & Catalysis (ELCAT))

#### Abstract

The electrochemical reduction of CO<sub>2</sub> into chemicals is considered to be a viable option for closing the carbon cycle. Although there is still room for improvement with respect to the individual components (i.e. electrocatalyst and membrane), important progress has been made in recent years, resulting in highly selective materials. However, so far, little attention has been given to the investigation and optimization of the ECR reactor design and process parameters, which are equally, if not more, important in order to up-scale the process towards an industrial level. For this reason, we have developed different types of CO<sub>2</sub> electrolyzers. First, we have elaborated on the implementation of convective flow inside the gas diffusion electrode (GDE) in comparison with a diffusive flow-by configuration. The pivotal role of operating on a CO<sub>2</sub> excess environment was established. Secondly, we have investigated the influence of the differential pressure across the GDE. Results show that by controlling the differential pressure at 0mbar, perspiration is minimal, leading to an overall FE of 76% over 6h at 100 mA/cm. Finally, we diminished voltage losses through a zero-gap configuration. It was demonstrated that water management in the GDE was crucial to avoid flooding and (bi)carbonate precipitation.

#### Biography: Tom Breugelmans

Prof. Tom Breugelmans is head of the research group Applied Electrochemistry and Catalysis (ELCAT) at the University of Antwerp. After obtaining his PhD in engineering in 2010, he was parttime professor at the Electrochemistry and Surface Engineering (SURF) group at the Vrije Universiteit Brussel between 2012 and 2017. Today, he is also affiliated as academic expert to VITO. Since 2016, he is Belgian representative of ISE. Currently, he is supervisor of 3 post-docs and promotor of 11 ongoing PhD studies. His main expertise is in the field of electrochemical techniques, electrocatalysis, electrosynthesis, reactor engineering and CO<sub>2</sub> reduction.

### 364 | Revisiting biomass wastes based-activated carbons in supercapacitors: Volumetric performance

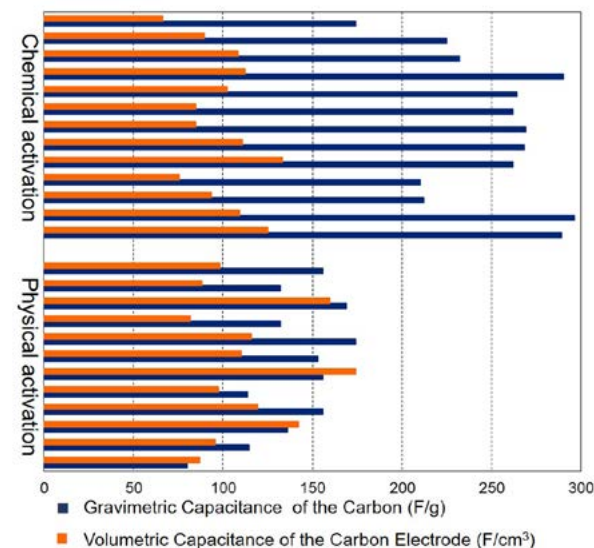
Teresa A. Centeno (Instituto de Ciencia y Tecnología del Carbono (INCAR-CSIC)), Loreto Suárez (Instituto de Ciencia y Tecnología del Carbono (INCAR-CSIC))

#### Abstract

Currently, a large number of studies is being devoted to biomass residues as precursors of lowcost porous carbons for supercapacitor electrodes. The majority involves activation by KOH and outstanding gravimetric capacitances are reported for the resulting carbons. However, the performance in volumetric terms, which is more relevant for practical implementation, is usually overlooked.

The assessment of a variety of carbons derived from solid residues generated in the industrial processing of grapes, apples and cherries reveals that simple activation by steam or CO<sub>2</sub> results to be a much more effective strategy for compact devices. The good balance of porosity and density displayed by physically activated carbons and their good packaging in electrodes allows enhancing the volumetric performance in aqueous electrolytes.

This study illustrates that the rational design of efficient carbons for supercapacitors has to be focused on the volumetric capacitance of the electrodes, rather than in the gravimetric or volumetric parameters of the materials. Additionally, the electrolyte contributions also have to be taken into account.



#### Biography: Teresa A. Centeno

Teresa A. Centeno obtained her PhD from the University of Oviedo, Spain, and is now Senior Researcher at Instituto de Ciencia y Tecnología del Carbono-CSIC. Her research encompasses preparation, characterization and application of carbons in energy-related processes and emissions reduction. Currently, her interests are focused in biomass wastes as source of high performance carbons and valuable compounds for energy and environmental applications.

### 565 | Optimization of the PEM fuel cells MEA preparation by depositing ultrasound dispersed catalytic ink on the membrane surface

Jakub Mališ (Department of Inorganic Technology, Faculty of Chemical Technology, University of Chemistry and Technology, Prague, Technická 5, Prague 6 – Dejvice, 166 28, Czech Republic), Veronika Markova (Department of Inorganic Technology, Faculty of Chemical Technology, University of Chemistry and Technology, Prague, Technická 5, Prague 6 – Dejvice, 166 28, Czech Republic), Martin Paidar (Department of Inorganic Technology, Faculty of Chemical Technology, University of Chemistry and Technology, Prague, Technická 5, Prague 6 – Dejvice, 166 28, Czech Republic), Karel Bouzek (University of Chemistry and Technology, Prague)

#### Abstract

Necessity of using platinum metals based catalysts represents one of the main drawbacks of the proton exchange membrane fuel cells (PEM FCs). Reduction of platinum loading thus represents necessity in order to make PEM FC technology economically competitive. One approach to the catalyst loading reduction represents deposition of the catalytic layer directly on the membrane surface, so called catalystcoated membrane (CCM). CCM technique provides excellent ionic contact between catalyst layer and polymer electrolyte. Catalyst utilisation is thus improved. The main problem this technique faces represents repeated membrane drying and humidification connected with changes in its dimensions. It potentially leads to the defects in the produced catalytic layer. The target of this study is to provide deeper insight into impact of parameters of the catalyst deposition on the MEA performance for membranes based on ionomer molecules of different structure. Properties of catalytic layer can be improved by using of ultrasonic nozzle for catalytic ink dispersion during the catalyst deposition process. It improves homogeneity of the catalyst distribution over the membrane surface and minimizes agglomeration of the catalyst particles. Properties of MEAs prepared on this way were compared with the commercial available electrodes.

#### Biography: Jakub Mališ

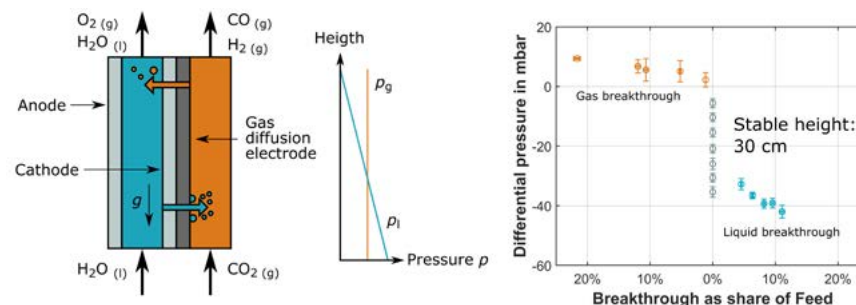
Jakub Malis, the presenting author, is a researcher at Department of Inorganic Technology, at University of Chemistry and Technology in Prague (UCT Prague). He defended Ph.D. thesis at the UCT Prague: "Pefluorinated sulfonated membranes as solid electrolyte for PEM water electrolysis in wide range of temperatures and pressures". His research is focused on the perfluorinated sulfonated membranes, PEM fuel cells, CCM, CCE, catalyst deposition, stack operation conditions.

### 312 | Scale-up limitation of gas diffusion electrodes for CO<sub>2</sub> conversion

Lorenz Baumgartner (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands), David Vermaas (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands)

#### Abstract

Electrochemical CO<sub>2</sub> reduction could decrease greenhouse gas emissions and store excess renewable electricity in the form of hydrocarbons. Delivering CO<sub>2</sub> in the gas phase through gas diffusion electrodes (GDE) can overcome mass transfer limitations imposed by the limited solubility and diffusion in the liquid phase. At a centimeter scale, industrially relevant current densities ( $\geq 300$  mA/cm<sup>2</sup>) have already been achieved in laboratory electrolyzers. At a larger scale, larger hydrostatic and/or hydrodynamic pressure gradients can emerge, which make the separation of liquid and gas phase challenging. Pressure gradients across the porous gas diffusion layer can lead to breakthrough of gas or liquid resulting in performance decrease and intermixing of the reaction streams. We aim to quantify the scale-up limitation imposed by the presence of pressure gradients in the liquid phase. We emulated a large scale system with a small scale setup by controlling the pressure gradient across the GDE and measuring the breakthrough behavior. We determined a stable pressure range of only 30 mbar ( $\approx 30$  cm height) for the commercial GDE substrate Sigracet 39BC. This result shows that it is necessary to improve the pressure stability of GDEs to make the scale-up of gas fed CO<sub>2</sub> electrolyzers more economical.



#### Biography: Lorenz Baumgartner

- 2018–Present PhD candidate, Delft University of Technology
- 2017-2018 Research Engineer, Massachusetts Institute of Technology
- 2014-2017 Master of Science, Technical University of Munich
- 2011-2014 Bachelor of Science, Technical University of Munich

### 301 | Energy efficient desalination with membrane capacitive deionization (MCDI): findings of theoretical and pilot studies

Ulrich Hellriegel (Laboratory of Industrial and Synthetic Organic Chemistry (LISOC), Department of Chemistry and Chemical Technologies, University of Calabria, Italy), Edgardo Cañas Kurz (Laboratory of Industrial and Synthetic Organic Chemistry (LISOC), Department of Chemistry and Chemical Technologies, University of Calabria, Italy), Alessio Caravella (Department of Computer Engineering, Modeling, Electronics and System Engineering, University of Calabria, Italy), Bartolo Gabriele (Laboratory of Industrial and Synthetic Organic Chemistry (LISOC), Department of Chemistry and Chemical Technologies, University of Calabria, Italy), Alberto Figoli (Institute on Membrane Technology, National Research Council (ITM-CNR), Italy), Jan Hoinkis (Center of Applied Research (CAR), Karlsruhe University of Applied Sciences, Germany)

#### Abstract

To make membrane capacitive deionization (MCDI) deployable for sustainable drinking water production, modular pilot scaled concepts and modelling strategies have been developed. Lab scale experiments demonstrate that an energy efficient desalination of brackish water is visible with commercial MCDI modules and can be a viable option compared to other desalination technologies. Salt solutions can be desalinated from 1000 mg L<sup>-1</sup> below 450 mg L<sup>-1</sup> with a specific energy consumption of SEC = 0.3 kWh m<sup>-3</sup>. Hereby, the mobility of different ions as well as the composition of the model water largely affects the removal efficiency. A developed FEM simulation model for CDI is being compared with the modified Donnan model, which can describe experimental data sufficiently, also when applied voltages at the module are low. For calculating specific energy consumption, RC models will be implemented. For desalinating brackish water with higher concentrations of salt, a combination process of low-pressure RO membranes and MCDI is tested at pilot scale in coastal area of Vietnam. Hereby, the MCDI module acts as polisher, compensating fluctuations of salt concentration which can occur in tropical coastal regions according to raining and dry seasons. The low-pressure concept allows a low-cost and easy to implement setup.

#### Biography: Ulrich Hellriegel

##### Academic Background:

- 2016 - present: University of Applied Sciences, Karlsruhe, Germany, Academical assistant in water treatment projects
- 2011 - 2014: University of Applied Sciences, Karlsruhe, Germany, Researcher in refrigeration, environmental engineering and fluid dynamics
- 2010 - 2011: SINTEF Energi AS, Trondheim, Norway, Researcher in CO2 air-conditioning technology

##### Research Interests:

- Novel water treatment-technologies
- Renewable energy
- Modelling and numerical simulation
- Fluid dynamics

##### Educational Background:

- 2017 - present: PhD student at University of Calabria, Italy, Department of Chemistry and Chemical Technologies
- 2014: University of Applied Sciences, Karlsruhe, Germany, Mechanical Engineering - Energy Efficiency, M.Sc.
- 2012: University of Applied Sciences, Karlsruhe, Germany, Mechanical Engineering- Refrigeration, Air- Conditioning and Environmental Engineering, B.Eng.

### 530 | Modeling of the two-phase transport in PEM fuel cell

Erwan Tardy (Univ. Grenoble Alpes, CEA, LITEN, DEHT), Jean-Philippe Poirot (Univ. Grenoble Alpes, CEA, LITEN, DEHT), Yann Bultel (Univ. Grenoble Alpes, CNRS, Grenoble INP, LEPMI, 38000 Grenoble, France), Pascal Schott (Univ. Grenoble Alpes, CEA, LITEN, DEHT), Christophe Morel (Univ. Grenoble Alpes, CEA, LITEN, DEHT), Guillaume Serre (Univ. Grenoble Alpes, CEA, LITEN, DEHT), Marion Chandesris (Univ. Grenoble Alpes, CEA, LITEN, DEHT)

#### Abstract

The Proton Exchange Membrane Fuel Cell (PEMFC) is a promising candidate for many applications, either stationary or transportation. Of the many barriers, cost and durability represent two of the most significant challenges to achieving clean, reliable and cost-effective fuel cell systems. Effective management of the liquid water and heat produced in PEM fuel cells remains crucial to increase both its performance and durability. A two-phase multi-component model of a PEM fuel cell is developed. The model considers the cell as a multilayered system and each layer is accurately in-plane discretized to allow the simulation of local temperature and species heterogeneities, including liquid water. The objective of the model is the prediction of the distributions of current density, species concentrations, water content and temperature in all the components of the cell, while taking into account the real flowfield designs. The model can be compared to experimental temperature and current density data and liquid water measurement obtained from neutron imaging tests in several operating conditions.

#### Biography: Erwan Tardy

My name is Erwan Tardy. I am currently a PhD student at CEA Grenoble. My work focuses on the modeling of a PEM fuel cell using the COMSOL Multiphysics software, and more particularly on the two-phase transport within the fuel cell.

**611 | Up-scaling a zero-gap CO<sub>2</sub> electrolyzer beyond the pilot scale**

Michiel Vranckaert (University of Antwerp), Jonas Hereijgers (Research group Applied Electrochemistry & Catalysis (ELCAT), University of Antwerp, Universiteitsplein 1, 2610 Wilrijk), Tom Breugelmans (University of Antwerp, Research Group Applied Electrochemistry & Catalysis (ELCAT))

**Abstract**

It is well known that for the past decades increasing CO<sub>2</sub> concentrations contribute to global warming. The electrochemical reduction of CO<sub>2</sub> offers a solution in this matter by utilizing waste CO<sub>2</sub> as a feedstock for the production of base chemicals, reducing harmful emissions in the process. The implementation of this idea into the structure of today's industry will lead to a transition towards a more circular economy. However, the feasibility of this solution is heavily dependent on the scale at which this electrochemical process can be executed.

In this work we developed a zero-gap PEM electrolyzer with a capability of 1kW, capable of performing CO<sub>2</sub> reduction at high current densities and low cell voltages in a stable fashion. An up-scaled single cell electrolyzer housing a GDE of 200cm<sup>2</sup> was constructed and tested. Our results show that operating at a current density of 100mA/cm<sup>2</sup>, a FE and CO<sub>2</sub> conversion of respectively 80% and 40% was achieved. Crucial herein [MV1] was the development of a novel water management system and careful tuning of the CO<sub>2</sub> flow distribution to tackle the emerging problems inherent to the upscale process. Implementing these solutions constitutes an important milestone regarding valorisation of CO<sub>2</sub> on an industrial scale.

**Biography: Michiel Vranckaert**

Industrial engineer and doctoral fellow at research group ELCAT (Applied Electrochemistry and Catalysis). Specializing in the design and principles of the next generation electrochemical reactors.

**270 | Ion-Dependent Capacitive Deionization with Porous Carbon Electrodes**

Joren Vos (Universiteit Utrecht), Danny Inder Maur (Universiteit Utrecht), Henrik Rodenburg (Universiteit Utrecht), Ben Ern  (Universiteit Utrecht)

**Abstract**

Capacitive deionization requires electrode materials with a high surface-to-volume ratio, implying pores that are hardly wider than the size of hydrated ions. By studying the uptake capacity of porous carbon electrodes for different aqueous salts, not only NaCl, we probe the porous network on the length scales of the sizes of different ions. Calorimetry performed during charging and discharging gives strongly different results depending on the type of counterion, and the reversible heat of double layer formation even has a different sign for sodium and chloride. Our earlier heat measurements (Phys. Rev. Lett. 119, 166002 (2017)) did not reveal this difference, since they were not done separately on cathode and anode and therefore were not ion-specific. Our tentative explanation of the heat effects is in terms of the different sizes of the hydrated ions on the entropy of the double layer. For a further test of this theory, we are presently implementing ion-specific in situ NMR spectroscopy, as a way to characterize the concentrations of the counterions and co-ions inside the pores.

**Biography: Joren Vos**

The author is currently doing his Ph.D. thesis on Experimental Thermodynamics of Ion Confinement in Porous Carbon Electrodes at the University of Utrecht under the supervision of Dr. Ben Ern .

## 286 | Effect of operation temperature on the performance of Hydrogen-Chlorine PEM Fuel Cells

Mireya Carvela (University of Castilla La Mancha), Sergio Díaz Abad (University of Castilla La Mancha), Justo Lobato (University of Castilla La Mancha), Manuel A. Rodrigo (University of Castilla-La Mancha)

### Abstract

Nowadays, technologies for efficient and environment-friendly energy production and storage have become paramount importance than at any time. In this work, the development of one of these new technologies is investigated: Hydrogen-Chlorine PEM fuel cell.

In particular, in the proposal research will be exposed the changes on the performance of Hydrogen-Chlorine PEM fuel cell working under different temperature conditions. Because of that, two different Proton Exchange Membrane (PEM) have been used, according to their high temperature-resistance: Nafion (25-80°C) and Polybenzimidazole (PBI) (100-160°C).

On these conditions, we have checked that the best results have been obtained by using the Nafion membrane working at room temperature (25°C). Furthermore, in this work, the fuel cell is fed with humidified hydrogen (gas) and chlorine (gas) in the anodic and cathodic compartment, respectively. The use of humidified chlorine has allowed to obtain more efficient results than the employment of non-humidified chlorine, in all operation conditions. Finally, the results are similar than the results obtained on chlor-alkali electro-absortion cells. For this reason, we can confirm that this new promising technology has a reliable efficiency.

### References

Financial support from the Spanish Ministry of Economy, Industry and Competitiveness and European Union through project CTQ2017-91190- EXP (AEI/FEDER, UE) is gratefully acknowledged.

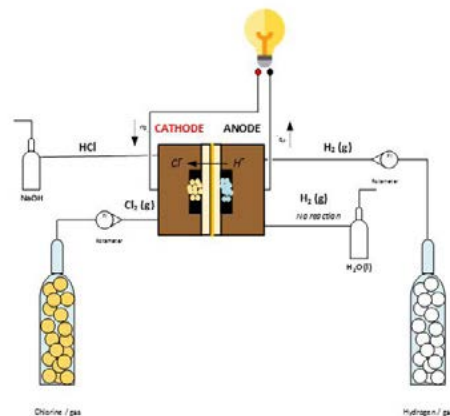
### Biography: Mireya Carvela

Mireya Carvela is a PhD student at the Department of Chemical Engineering, University of Castilla-La Mancha (Spain).

She finished a degree in Chemical Engineering at University of Castilla-La Mancha, where she also obtained two masters: Master in Chemical Engineering and Master in Environmental Engineering and Management.

She has research experience in the development of electrochemical technologies, reached during her investigation work at University of Castilla-La Mancha in the last years.

At the present time, she researches a new environment-friendly way to produce and store electrical energy: reversible Hydrogen-Chlorine cells.



## 278 | Up-scaling zero gap continuous-flow electrolyzer cells for the electrochemical reduction of carbon-dioxide

Balázs Endrődi (University of Szeged, Department of Physical Chemistry and Materials Science), Egon Kecsenovity (University of Szeged, Department of Physical Chemistry and Materials Science), Angelika Samu (University of Szeged, Department of Physical Chemistry and Materials Science), Csaba Janáky (University of Szeged, Department of Physical Chemistry and Materials Science)

### Abstract

Either considering carbon dioxide as a feedstock for transportation fuels and commodity chemicals or aiming to reduce its atmospheric emission, electrochemical reduction of CO<sub>2</sub> is one of the major scientific and engineering challenges. To match the requirements of industrial implementation, this reaction must proceed with high energy efficiency, reaction rate and selectivity simultaneously, which can be achieved in continuous-flow electrolyzers. Rapidly increasing amount of experimental data using such (laboratory-scale) devices is available in the scientific literature, but, following the footsteps of the PEM water electrolysis society, the subsequent inevitable phase in the technological evolution is the up-scaling of these to larger size. In this presentation we demonstrate a possible up-scaling pathway for zero-gap electrolyzers by assembling multiple electrolyzer units in a single cell. The inner structure of the device is designed so to allow parallel or serial connection among the electrolyzer units with regards to the carbon dioxide feed. This way the operation of the cell (reaction rate, conversion efficiency) can be tailored to the specific requirements of the applied product stream processing technology. The effect of different operation conditions on the reaction rate and selectivity will be discussed during the presentation.

### Biography: Balázs Endrődi

Balázs Endrődi (born 1987. 11. 25.) works as an assistant professor at the Department of Physical Chemistry and Materials Science of the University of Szeged, Hungary. His current research focuses on the electrochemical reduction of carbon dioxide, and on the possible up-scaling of this technology to match the industrial needs. His research interest also covers other industrially relevant electrochemical processes, e.g. PEM water electrolysis or electrolytic chlorate production, mostly focusing on the selectivity, energy efficiency and sustainability of these. He is the co-author of 36 scientific publications, with a cumulative impact factor above 200 and with above 600 citations.

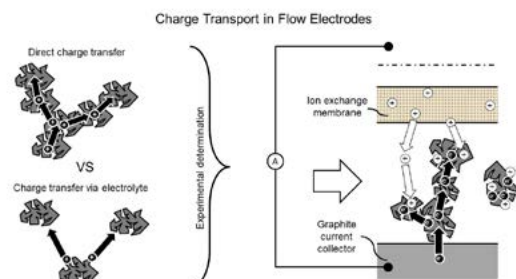


## 87 | Particle Interaction in Slurry Electrodes Influencing the Charge Transport in Flow-Electrode Capacitive Deionization

Christian Linnartz (DWI - Leibniz-Institute for interactive materials e.V.), Maria Padligur (RWTH Aachen University, Aachener Verfahrenstechnik-Chemical Process Engineering), Felix Stockmeier (RWTH Aachen University, Aachener Verfahrenstechnik-Chemical Process Engineering), Korcan Percin (DWI - Leibniz-Institute for interactive materials e.V.), Matthias Wessling (RWTH Aachen University, Aachener Verfahrenstechnik-Chemical Process Engineering and DWI - Leibniz-Institute for interactive materials e.V.)

### Abstract

In the future, electrochemically driven reactions or separation processes will complement most of today's processes driven by pressure or heat. Flow electrodes have become of great interest in electrochemical applications in recent years since they increase the active surface by complex flow. Flow electrodes are well applicable in selective desalination, treatment of contaminants in wastewater, fuel synthesis, and energy storage. By flowing over a working electrode, the particles are charged and can be used for faradaic and nonfaradaic surface reactions, like capacitive ion storage or electrochemical synthesis. The exact path of charge transfer both between the particles and between particles and working electrode is a topic of ongoing research. The present work will unravel new details by direct combination of an electrical and optical analysis of the complex flow regimes. To achieve this, we apply a microfluidic setup in combination with high-speed visualization and electrochemical measurements. The influence of electrical charge percolation via direct particleparticle contact versus ion diffusion in the surrounding electrolyte is discussed in detail. Charge transport in laminar boundary layers or electrode particle interactions can be distinguished from phenomena in the bulk phase of the flow electrodes. En route for application, these knowledge gaps shall be closed.



### Biography: Christian Linnartz

#### EDUCATION

- 2016 - present PH.D. STUDENT at DWI - Leibniz- Institute for interactive Materials, Aachen (DE), Chair of Chemical Engineering at RWTH Aachen University (DE) Supervision: Prof. Dr.-Ing. Matthias Wessling
- 2016 MASTER OF SCIENCE at Technion - Israel Institute of Technology, Haifa (IL) and Chair of Chemical Engineering at RWTH Aachen University (DE)

#### PUBLICATIONS

- C J LINNARTZ, A Rommerskirchen, M Wessling, Y Gendel; ACS Sustainable Chemistry & Engineering 5 (5), 2017, 3906-3912
- A Rommerskirchen, C J LINNARTZ, M Wessling; ACS Sustainable Chemistry & Engineering 6 (10), 2018, 13007-13015
- A Rommerskirchen, A Kalde, C J LINNARTZ, M Wessling, Carbon 145, 2019, 507-520

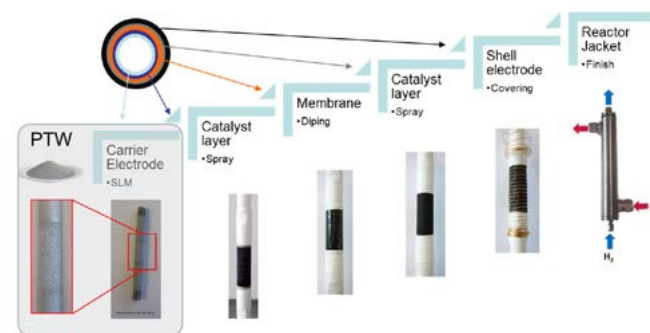
## 25 | Challenges in developing tubular high-temperature proton exchange membrane fuel cells (HT-PEM-FCs)

María Catalina Bermúdez Agudelo (Thermal Process Engineering Group (TVT) | Technische Universität Darmstadt), Manfred J. Hampe (Thermal Process Engineering Group (TVT) | Technische Universität Darmstadt)

### Abstract

The high energy demand combined with the ambitious gas emissions objectives create a scenario for green and efficient energy production methods. Fuel cell technology is a promising alternative to generate electrical and thermal energy with harmless emissions. Among the fuel cell devices, the high-temperature (HT) proton exchange membrane (PEM) fuel cells (FCs) have been actively investigated due to the benefits compared with their low-temperature (LT) counterparts in both stationary and non-stationary applications.

The predominant design studied for HT-PEM-FC corresponds to the conventional planar-frame structure. As a result, significant advances using this shape have been reached. However, studies using a tubular geometry in LT-PEM-FC showed improvements in the power density, which makes this non-conventional design an attractive possibility for future developments. The transfer of this tubular type to HT-PEM-FCs has been attempted by our institute in recent years. This paper provides an overview of the challenges faced in the design of the compact and robust arrangement presented in Figure 1, such as customization of gas diffusion layers (GDLs), MEA preparation, fuel cell fixation and electrical connection, as well as the future plans for the proposed tubular fuel cell.



### Biography: María Catalina Bermúdez Agudelo

María Catalina Bermúdez Agudelo is a researcher in the topic of tubular high temperature proton exchange membrane fuel cells at the Technische Universität Darmstadt. She received a bachelor's degree in chemical engineering from the Pontifical Bolivarian University and a master's degree in "Utilities and Waste - Sustainable Processing" from Karlsruhe Institute of Technology. She has professional experience as a researcher and manager and hands-on experience in laboratory work. Her current project includes the manufacturing, characterization, and modeling a novel fuel cell using a 3D-printed metallic porous anode Gas Diffusion Layer.

**Plenary: Electrocatalysis beyond surface reaction energetics**

*Karen Chan, Technical University of Denmark, Denmark*

Beyond surface reaction energetics, the structure and composition of the electric double layer exerts an influence on the activity and selectivity of electrochemical reactions. In this talk, I first discuss the impact of the electrolyte on electrocatalytic activity from the perspective of the impact of the proton donor and adsorbate dipole-field interactions, as well as how cations and supported single site catalysts tune the latter. I then discuss the impact of solution phase reactions and mass transport on activity and selectivity. I draw examples from hydrogen evolution and electrochemical CO<sub>2</sub> reduction, and discuss the implications of fundamental mechanistic understanding on catalyst design.

**616 | Toward market implementation of CO<sub>2</sub> electrochemical reduction to formic acid**

*Dr. Louis Legrand (Coval Energy), Mr. Rien van Haperen (Coval Energy), Mr. Robert de Kler (Coval Energy), Dr. Mariette de Groen (Coval Energy)*

**Abstract**

Reducing CO<sub>2</sub> emissions is one of the greatest challenges of this century to limit the effect of global warming. CO<sub>2</sub> capture and utilization and storage (CCUS) is a promising route to convert unwanted CO<sub>2</sub> emissions into valuable carbon product. Coval energy contribute to CCUS by developing technology converting CO<sub>2</sub> into formic acid, and by collaborating with partners to develop complete CO<sub>2</sub> value chain based on formic acid (see Figure 1). The “Coval” technology is based on high pressure CO<sub>2</sub> pressure electrolyzer, a technology in which only electrical energy is required that facilitates its integration with renewable energy. Our recent research work shows that using high CO<sub>2</sub> pressure improve the CO<sub>2</sub> reduction performance by (i) increasing the faraday efficiency and (ii) increasing the current density. Our current work is focusing on upscaling this technology to pilot-scale in combination with CO<sub>2</sub> capture to demonstrate the technology maturity, and participate to the demonstration of CO<sub>2</sub> reduction technology in general.

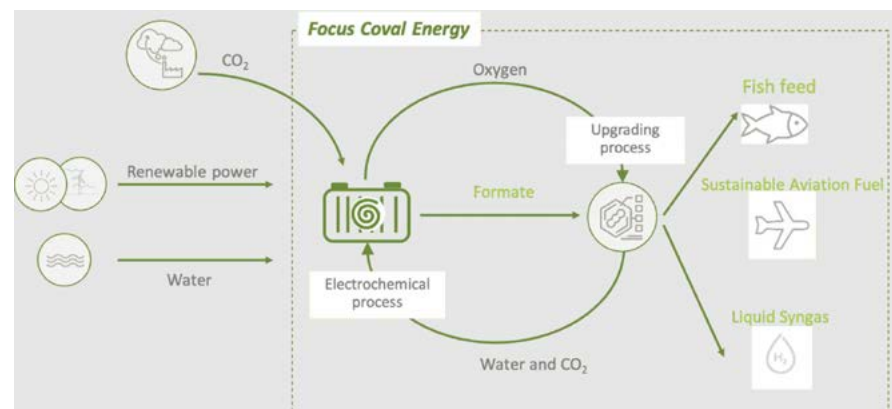


Figure 1: Focus on technology development of Coval Energy (<https://www.covalenergy.com/>)

**Biography: Louis Legrand**

Louis Legrand is the R&D manager in Coval Energy, where he is in charge of developing the electrochemical CO<sub>2</sub> conversion into formic acid technology. Previously, he co-developed a CO<sub>2</sub> capture based on supercapacitors at Wetsus during his PhD project. Strong of his experience on both CO<sub>2</sub> capture and conversion fields, his main vision is to develop both technologies toward market to actively contribute to CCUS in order to reduce CO<sub>2</sub> emissions.

## 542 | Tween 80 enhanced electrochemical remediation of phenanthrene contaminated groundwater containing high chloride content

Fei Miao (Wuhan University), Fuzhen Liu (Wuhan University, China), Yin Xu (Wuhan University, China), Zhengzhi Liu (Wuhan University, China), Yanyan Ma (Wuhan University, China), Jinjin Zhao (Wuhan University, China), Hui Zhang (Wuhan University)

### Abstract

In situ chemical oxidation (ISCO) has been widely applied for the remediation of contaminated soil and groundwater. However, it usually suffers from lower removal efficiency of contaminants from groundwater due to the hydrophobicity and slow dissolution or desorption rates of dense nonaqueous phase liquids (DNAPLs). Surfactants can reduce the interfacial tension between the DNAPLs and the aqueous phase for their amphiphilic properties and increase the solubility of DNAPLs. Herein, in the presence of high concentration of chloride, an effective technology was proposed to generate active chlorine through electrolysis for the oxidation of phenanthrene (PHE) with the assistance of surfactant Tween 80 (TW-80). The introduction of 50 mM NaCl successfully accelerated the abatement of PHE to 95.9% within 90 min in the presence of 5 g L<sup>-1</sup> TW-80 at 0.5 A of applied current. The detection of active chlorine species and scavenging experiments indicated that the dominated active species involved in the PHE abatement were active chlorine and hydroxyl radicals ( $\cdot\text{OH}$ ) generated at the DSA anode. This research pioneers a novel alternative process (EO/Cl<sup>-</sup>) for PHE-contaminated groundwater remediation when containing surfactants.

### Biography: Fei Miao

Fei Miao, who is a PhD candidate from Wuhan University, China. Her main research is contaminants removal via electrochemical advanced oxidation processes.

## 612 | Conductivity of LSM-YSZ layer for thickness of active electrode zone identification

Daniel Budáč (University of Chemistry and Technology, Prague), Michal Carda (University of Chemistry and Technology, Prague), Martin Paidar (University of Chemistry and Technology, Prague), Karel Bouzek (University of Chemistry and Technology, Prague)

### Abstract

Solid oxide cells (SOCs) serve as efficient energy conversion devices. Mixture of La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3-δ</sub> and ZrO<sub>2</sub>-Y<sub>2</sub>O<sub>3</sub> (LSM-YSZ) represents oxygen electrode material commonly used in SOC. It is widely known that content of YSZ in the material leads to extension of active electrode zone by introducing ion conductive phase leading to increased probability of three phase boundary occurrence. Contrarily, electric resistance of LSM-YSZ material increases with YSZ content, since YSZ is two orders of magnitude less conductive than LSM. Detailed information on YSZ content influence on extension of the electrode active zone is, however, scarce in the literature. It was already proved that optimal ratio of LSM:YSZ in electrode in terms of SOC performance is 1:1; however, it leads to significant decrease of electrode conductivity in comparison to pure LSM. This effect has to be considered, when experimental data are evaluated, especially with regard to kinetic parameters evaluation. Goal of this study is to quantify impact of YSZ content on LSM-YSZ conductivity. Using the data obtained, mathematical model will allow calculation of local potential and current distribution in oxygen electrode in SOC.

### Acknowledgements

The authors acknowledge the financial support of the Czech Science Foundation (GACR), contract No: 19-142-44-J and Specific university research (A2\_FCHT\_2021\_083).

### Biography: Daniel Budáč

Daniel Budáč, the presenting author, is a Ph.D. student at Department of Inorganic Technology, at University of Chemistry and Technology in Prague. He graduated from the University of Chemistry and Technology in Prague in the study program: "Hydrogen and Membrane Technologies" (diploma thesis: "Properties of oxygen electrode in solid oxide reversible cell"). His Ph.D. research is focused on the high temperature electrochemical reactors for energy storage such as high temperature solid oxide cells.

## 602 | Using bi-layer membranes to prevent drying-out during CO<sub>2</sub> Electrolysis

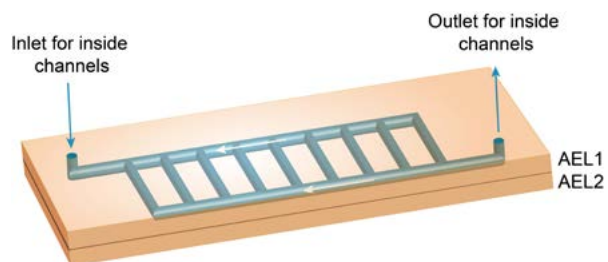
Kostadin Petrov (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands), Justin Bui (Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, California, 94720-1462), Alexis Bell (Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, California, 94720-1462), Adam Weber (Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, California, 94720-1462), David Vermaas (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands)

### Abstract

Large-scale CO<sub>2</sub> electrolysis could allow the sustainable production of fuels and chemicals while offering a means to store renewably generated energy. Nonetheless, a major obstacle in the development of CO<sub>2</sub> electrolyzers is that they tend to dry-out as water is consumed in the CO<sub>2</sub> reduction reaction, which infinitely increases resistance due to a less conductive medium. Therefore, there is a demand to develop improved strategies to maintain water balance.

This project aims to tackle this challenge by using the novel concept of a bi-layer ion-exchange membrane (IEM). This membrane has small channels between the two layers, which allow the circulation of water or an electrolyte. In our work, the relationship between the presence of water, different concentrations of KHCO<sub>3</sub> within the channels, and membrane conductivity during CO<sub>2</sub> electrolysis is studied, both numerically and experimentally.

According to initial modelling results, the presence of the channel inside the membrane can have a significantly positive effect on the water content and conductivity of the membrane-electrode assembly at high current density. Since water management is one of the keys for stable electrochemical CO<sub>2</sub> reduction, this method of ensuring that the membrane remains conductive during operation could aid in making the scale-up of this process possible.



### Biography: Kostadin Petrov

Currently, I am a PhD Candidate in the Transport Phenomena group, of the Chemical Engineering department of TU Delft. I'm working on nanoporous alkaline-stable membranes for CO<sub>2</sub> Electrolysis. Previously, I completed an MSc course in Chemical and Biochemical Engineering in the Faculty of Science and Technology of NOVA University of Lisbon, and did my MSc thesis work in TU Delft as an exchange student. After graduating, I worked for 6 months under a junior researcher scholarship by REQUIMTE in the "BioRevinery" project, where I performed extractions using supercritical CO<sub>2</sub>.

## 459 | Is electro-assisted leaching a feasible option for the recovery of trace elements from municipal solid waste incinerator bottom ash?

Sahar Belfqueh (Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, LEPMI, Grenoble, France), Jonathan Deseure (Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, LEPMI, Grenoble, France), Maria-Octavia LUPSEA TOADER (University of Lyon, INSA-Lyon, DEEP Laboratory, Villeurbanne, France), Denise Blanc (University of Lyon, INSA-Lyon, DEEP Laboratory, Villeurbanne, France), Christine De Brauer (University of Lyon, INSA-Lyon, DEEP Laboratory, Villeurbanne, France), Lenka Svecova (Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, LEPMI, Grenoble, France)

### Abstract

In the E.U., Norway and Switzerland nearly 90 Mt of municipal solid waste are incinerated each year producing over 17 Mt of Municipal Solid Waste Incineration Bottom Ash (MSWI-BA). This study focuses on alternative ways of MSWIBA valorisation, namely the recovery of trace elements with a double objective: (i) to recover economically important metals and (ii) to pretreat bottom ash, before further valorisation/disposal. The efficiency of classical acid leaching is compared to the so-called electroassisted leaching. This innovative process is based on electrolysis of leaching solution to achieve the recovery and reuse of acids. Two different experimental set-ups were described in literature. Either the waste material is directly used as sacrificial anode and the applied potential is chosen to obtain the selective oxidation and dissolution of the target metals (direct leaching) or the solid material is put in suspension into an electrolyte and the leaching species are generated at the electrode-electrolyte interface (indirect leaching, used in this study). This study showed that for identical experimental conditions the indirect electro-assisted approach results in a significant enhancement of Cu and Zn leaching efficiency, compared to acid leaching, i.e. Cu leaching efficiency increased from 55% to 75% and Zn from 23% to 91%.

### Biography: Lenka Svecova

- Assistant professor at Grenoble Institute of Technology, researcher at the Laboratory of Electrochemistry and Physico-chemistry of Material and Interfaces (LEPMI UMR 5279) since 2008.
- Teaching activities: Unit operations, Sustainable development, Green chemistry and green chemical engineering, Safety and risk assessment, Life cycle assessment and eco-design, End-of-life and recycling, Recovery of metals
- Research activities: Recycling, Recovery of metals, Life cycle assessment, ion exchange, leaching, liquid-liquid extraction

## 193 | Anodic Oxidation of Iodobenzene Derivatives

Balamurugan Devadas (University of Chemistry and Technology, Prague, Dep. of Inorganic Technology), Jaroslav Kvicala (University of Chemistry and Technology, Prague, Dep. of Organic Chemistry), Martin Krupicka (University of Chemistry and Technology, Prague, Dep. of Organic Chemistry), Jan Svoboda (University of Chemistry and Technology, Prague, Dep. of Organic Technology), Tomas Bystron (University of Chemistry and Technology, Prague, Dep. of Inorganic Technology)

### Abstract

Oxidation of iodobenzene and its derivatives may yield hypervalent iodine compounds. Numerous representatives of this group of compounds are being used as mild oxidation agents in organic synthesis. Their main advantages are high selectivity, low toxicity and environmental friendliness. This represents a huge advantage compared to classical selective oxidants based usually on heavy metal ions. However, traditional approach towards synthesis of hypervalent iodine compounds is based on application of chemical oxidants such as peracids and/or their salts. Their application is connected with inherent safety issues and generation of the respective end oxidant reduction products. This increases price and limits accessibility as well as range of potential applications of hypervalent iodine oxidants. An alternative procedure obviating the need for the end oxidant application is anodic oxidation of iodobenzenes.

In the present contribution, recent advances in hypervalent iodine electrochemical synthesis in both the aqueous and nonaqueous environments achieved in our group will be summarised.

### References

The work was supported from European Regional development Fund-Project "Organic redox couple based batteries for energetics of traditional and renewable resources (ORGBAT)" No. CZ.02.1.01/0.0/0.0/16\_025/0007445.

### Biography: Tomas Bystron

Tomas Bystron is interested in electrochemical synthesis of organic compounds, hydrogen economy-related topics, electrocatalysis and biosensors development. He graduated and continues working at University of Chemistry and Technology Prague in Czech Republic. He finished his Ph.D. in 2009, in 2019 he was appointed associate professor of inorganic technology. During his studies and carrier he spent some time in laboratories abroad, namely at NTNU in Norway (prof. R. Tunold), ENSIC/CNRS in France (prof. F. Lapicque) and Imperial College London in United Kingdom (prof. G. Kelsall).

## 405 | Electroreduction of carbon dioxide on Cu-based mixed-metal oxide catalysts: tuning of syngas composition

Hilmar Guzmán (CREST group, Department of applied science and technology (DISAT), Politecnico di Torino and Center for Sustainable Future Technologies, IIT@Polito, Istituto Italiano di Tecnologia.), Daniela Roldán (CREST group, Department of applied science and technology (DISAT), Politecnico di Torino.), Micaela Castellino (CREST group, Department of applied science and technology (DISAT), Politecnico di Torino.), Nunzio Russo (CREST group, Department of applied science and technology (DISAT), Politecnico di Torino.), Simelys Hernández (CREST group, Department of applied science and technology (DISAT), Politecnico di Torino and Center for Sustainable Future Technologies, IIT@Polito, Istituto Italiano di Tecnologia.)

### Abstract

Electrochemical Reduction of CO<sub>2</sub> (ER-CO<sub>2</sub>) is a very attractive alternative to tackle Global Warming. Out of the various materials, copper performance is among the best achieved for CO<sub>2</sub> electroreduction to > C1+ products. In this work, catalysts with different Cu, Zn and Al amounts were synthesized by co-precipitation method. These kinds of catalyst are traditionally used for the CO<sub>2</sub> hydrogenation to CO and methanol at high temperature and pressure but, herein, they were tested for the first time for the ER-CO<sub>2</sub> under ambient conditions. The role on the performance of the catalysts of their morphology, chemical-physical properties and composition was studied by different characterization techniques (e.g. XRD, XPS, BET, etc) and electrochemical impedance spectroscopy at different applied potentials. Adding metal oxides, like ZnO and Al<sub>2</sub>O<sub>3</sub>, to the Cu catalyst contributed to promote CO formation over H<sub>2</sub>. The results reveal that by increasing the applied-potential, CO current density increase considerably in the case of mixed-metal oxide catalysts (see Figure 1). In fact, a tunable H<sub>2</sub>/CO ratio was achieved with the tricomponent catalyst. The so-obtained syngas can be used directly as a feedstock for the generation of numerous energy-dense chemicals in well-established processes. Further efforts are on-going to obtain commercially-relevant current densities.

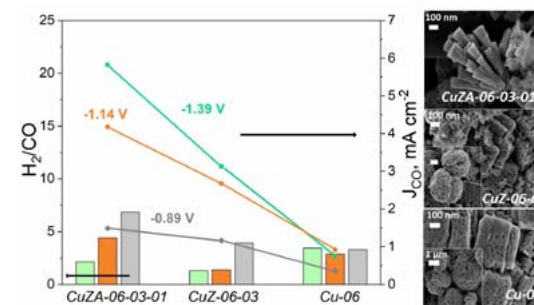


Fig. 1: H<sub>2</sub>/CO ratio and corresponding CO current density (J<sub>CO</sub>) at different working potentials and FESEM images of the mixed-metal oxide catalysts.

### Biography: Hilmar Guzmán

Hilmar Guzmán is 28 years old. She is Venezuelan. She has completed her master's degree and bachelor's degree at Politecnico di Torino (Italy), in the framework of a double degree between Politecnico di Torino (Italy) and Universidad Central de Venezuela (Venezuela). She is currently in the third year of her PhD course, which is focused in the conversion of CO<sub>2</sub> through an electrocatalytic route. She does her job with professionalism and responsibility, respecting the time needed to deliver the work and demonstrating problem solving skills.

### 303 | Ferrates(VI) and Environment

Jan Hives (Slovak University of Technology in Bratislava), Kamil Kereš (Slovak University of Technology), Emília Kubiňáková (Slovak University of Technology), Miroslav Gál (Slovak University of Technology)

#### Abstract

The high oxidation potential of ferrate(VI) may result in the most effective oxidizing agent. It was confirmed that ferrates are able to effectively degrade even very stable inorganic and organic pollutants. The oxidation of organic pollutants and microorganisms was accompanied by the disinfection properties of ferrate.

Ferrate is a strong, non-toxic oxidant with almost no harmful by products [1]. It is potentially an environmental friendly cleaner for both waste water and drinking water treatment. Therefore, effective means of the preparation of ferrate become a challenging task for several research groups all over the world [2].

In this study the electrochemical preparation of ferrate in strong alkaline environment at elevated temperatures is described. Various hydroxide electrolytes, anode materials and potentials were used [3].

The second part of this contribution was to monitor an interaction of ferrates with bacteria from natural water sources. Effect of ferrates was studied experimentally (a) on cyanobacteria species *Anabaena flosaquae*, (b) on real samples of surface water from natural water source Šaštín- Gazárka with occurrence of cyanobacteria, (c) on cyanotoxin microcystin-LR which is the most common toxin produced by cyanobacteria. Based on the results the significant degradation rate of cyanobacteria cell was proved at low ferrate concentration [4].

#### Biography: Jan Hives

Director of Institute of Inorganic Chemistry, Technology and Materials, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava from 2010.

- Member of Slovak Chemical Association
- Member of International Society of Electrochemistry
- Member of WPEE - EFCE
- Member of Scientific Board of FCHPT, Scientific Board of STU Bratislava, Scientific Board of FCHT VŠCHT Prague, Scientific Board of UACH-SAV Bratislava, Scientific Board of FMT VŠB TU Ostrava

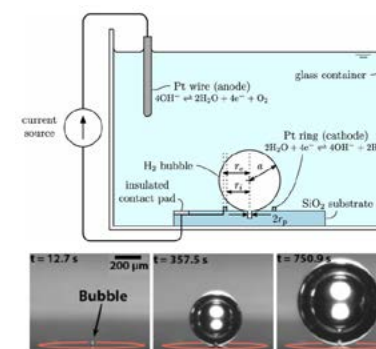
### 98 | Electrolytic gas bubble evolution on a hydrophobic cavity

Akash Raman (Mesoscale Chemical Systems, MESA+ Institute, University of Twente), Pablo Peñas Lopez (Physics of Fluids Group and Max Planck Center Twente, MESA+ Institute and J. M. Burgers Centre for Fluid Dynamics, Faculty of Science and Technology, University of Twente), Devaraj van der Meer (Physics of Fluids Group and Max Planck Center Twente, MESA+ Institute and J. M. Burgers Centre for Fluid Dynamics, Faculty of Science and Technology, University of Twente), Detlef Lohse (Physics of Fluids Group and Max Planck Center Twente, MESA+ Institute and J. M. Burgers Centre for Fluid Dynamics, Faculty of Science and Technology, University of Twente), Han Gardeniers (Mesoscale Chemical Systems, MESA+ Institute, University of Twente), David Fernández Rivas (Mesoscale Chemical Systems, MESA+ Institute, University of Twente)

#### Abstract

Bubbles influence mass transport at electrode surfaces in several electrolytic processes such as water splitting. A specific example is the increase of overpotential losses due to bubble coverage on electrodes, which is generally considered undesirable. To gain knowledge about the governing principles of bubble behavior on electrode surfaces and their influence on overpotential losses, our group is studying the nucleation, growth and detachment of successive electrolysis-driven bubbles on a hydrophobic micron-sized cavity surrounded by a ring microelectrode as shown in the image<sup>1</sup>. The cavity acts as a nucleation site for bubbles and prevents the coverage of the microelectrode at constant currents less than 50  $\mu\text{A}$ . This allows the study of single bubble growth and detachment during constant current experiments in a controlled manner. Previous work has theorized that bubbles may lower the concentration overpotential by decreasing the dissolved hydrogen concentration near the electrode. We demonstrate this effect by combining experiments with quasi-steady state diffusion models. Our electrode design offers new possibilities to observe the effect of bubbles on overpotential. This improved understanding will enable us to design more efficient gas-evolution electrodes.

<sup>1</sup>Pablo Peñas et al 2019 J. Electrochem. Soc. 166 H769 <https://doi.org/10.1149/2.1381914jes>



Pablo Peñas et al 2019 J. Electrochem. Soc. 166 H769 DOI: 10.1149/2.1381914jes

#### Biography: Akash Raman

Akash obtained his bachelor's degree in Chemical Engineering from SASTRA University, India and spent 6 months as a student research scholar at New York University. He then worked as a researcher at the Indian Institute of Technology Madras. He is currently a PhD candidate in the Mesoscale Chemical Systems (MCS) group at the University of Twente and his work focuses on understanding electrolysis driven bubble phenomena.

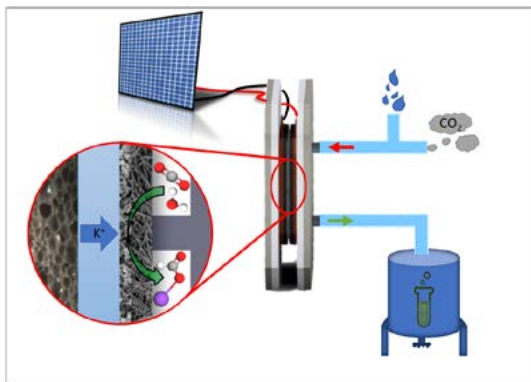
## 258 | The importance of water management in Zero-Gap CO<sub>2</sub> Electrolyzers

Bert De Mot (Research group Applied Electrochemistry & Catalysis (ELCAT), University of Antwerp), Jonas Hereijgers (Research group Applied Electrochemistry & Catalysis (ELCAT), University of Antwerp, Universiteitsplein 1, 2610 Wilrijk), Tom Breugelmans (University of Antwerp, Research Group Applied Electrochemistry & Catalysis (ELCAT))

### Abstract

The past decade, electrochemical reduction of CO<sub>2</sub> has received significant attention by the academic community and tremendous effort have been put into optimizing the electrolyser design. Current state-of-the-art electrolyzers are of the zero-gap type in which a gas-diffusion-electrode (GDE) is pressed directly against a membrane resulting in a membrane electrode assembly. In such zero-gap electrolyzers water management plays a crucial role in the performance of the electrolyser.

In this work, a zero-gap flow electrolyzer with a tin-coated GDE as cathode was used to convert humidified gaseous CO<sub>2</sub> to formate. The influence of humidification, CO<sub>2</sub> flow rate, flow pattern and the type of membrane on the Faradaic efficiency (FE), product concentration, and salt precipitation were investigated. It was demonstrated that water management in the GDE was crucial to avoid flooding and (bi)carbonate precipitation, which is of absolute importance if one wants to uphold a high FE and formate concentration. Direct water injection was validated as a novel approach for water management inside the electrolyser. At 100 mA/cm<sup>2</sup>, the direct water injection method in combination with an interdigitated flow channel resulted in a FE of 80% and an unprecedented formate concentration of 65.4 +/- 0.3 g/l without salt precipitation.



### Biography: Bert De Mot

Bert De Mot is a PhD-student in the research group Applied Electrochemistry & Catalysis at the University of Antwerp, Belgium. His main research is focussed on the electrochemical CO<sub>2</sub> reduction, converting CO<sub>2</sub> in useful products such as formate or carbon monoxide. Rather than optimizing the electro catalysts used in this process, he studies the influence of reactor engineering and process optimization on the overall efficiency and selectivity of the process.

## 682 | Electrochemical engineering of redox-active systems for integrating separations and reactions

Prof. Xiao Su (Chemical and Biomolecular Engineering, University of Illinois Urbana-Champaign Urbana, IL, 61820, United States)

### Abstract.

Separation processes play a critical role in water purification, carbon dioxide mitigation, and advanced chemical and biomolecular manufacturing. Electrochemical approaches present a sustainable alternative to traditional thermal and pressure-based methods, by regulating kinetics and thermodynamics based solely on electrical control. Redox-active interfaces offer an attractive platform for performing selective electrochemical separations. In particular, electroactive redox-polymers offer a wealth of flexibility in terms of functional group design, and control of electronic properties. First, we discuss the design of electrochemically-driven binding interactions in metallopolymers for selective anion capture, and the molecular tuning of the charge-transfer interactions. Second, redox-electrodes are leveraged towards tandem reaction and separations of target molecules. By asymmetric electrochemical design, electrosorbents and electrocatalysts can enable reactive separation within the same device, for the remediation of contaminants of emerging concern such as heavy metals and organic micropollutants, including perfluoroalkyl substances (PFAS). Finally, we present new approaches for critical metal recovery and waste recycling, through structural control and tunability of charge-transfer interactions.

These concepts point towards emerging directions in electrochemical interface design: by superimposing properly tuned chemical interactions onto electrostatics we can reach achieve unique molecular selectivity, and through judicious electrochemical engineering, even couple reaction and separation processes by electron-transfer.

### 31 | Photocatalytic nitrogen fixation: Prospects for Distributed Fertilizer Production

Marta Hatzell (Georgia Institute of Technology), Yu-Hsuan Liu (Georgia Institute of Technology)

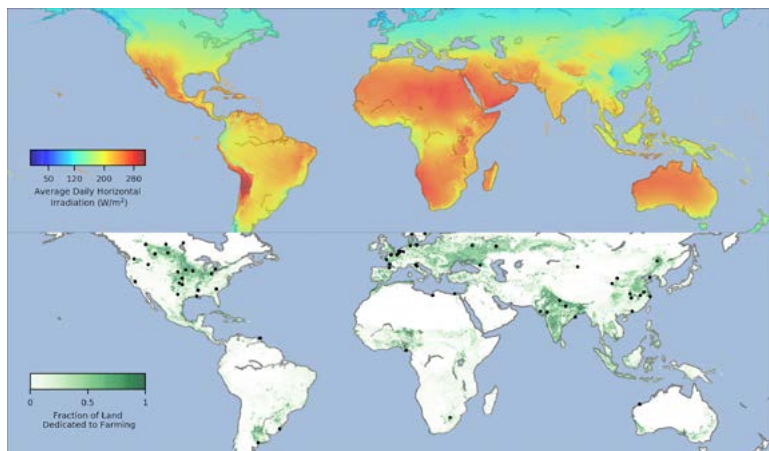
#### Abstract

Photocatalytic nitrogen fixation is a form of artificial photosynthesis capable of enabling distributed production of fixed nitrogen at nearambient conditions from the nitrogen, water, and photons that are readily available from the environment[1]. The process has been demonstrated over titania catalysts through both reductive and oxidative pathways, although the currently observed nitrogen fixation rates are too low to be practical for fertilizer synthesis[2]. Interestingly, the process occurs under environmental conditions and has been speculated to play a significant role in the global nitrogen cycle owing to the prevalence of  $\text{TiO}_2$  in naturally occurring sands. Despite the wide-ranging potential impacts of this reaction, the process has received relatively little attention and has not been studied with modern techniques. Here, through the use of advanced in situ surface science we provide new insight into the potential active site and reaction mechanism for nitrogen on titania. We will also detail the future engineering challenges which exist for solar fertilizer production.

#### References

[1] Medford, Andrew J., and Marta C. Hatzell. *\_Acs Catalysis\_*, 7, (2017).

[2] Comer, Benjamin M., Porfirio Fuentes, Christian O. Dimkpa, Yu-Hsuan Liu, Carlos A. Fernandez, Pratham Arora, Matthew Realf, Upendra Singh, Marta C. Hatzell, and Andrew J. Medford. *\_Joule\_* (2019).



#### Biography: Marta Hatzell

Marta Hatzell is an Assistant Professor of Mechanical Engineering at Georgia Institute of Technology. Prior to starting at Georgia Tech in August of 2015, she was a Post-Doctoral researcher in the Department of Material Science and Engineering at the University of Illinois - Urbana-Champaign, and she completed her PhD at Penn State University in 2014. Dr. Hatzell was awarded the NSF Early CAREER award in 2019 for her work on distributed solar-fertilizers.

### 681 | Nanopore-Based Power Generation from Salinity Gradient: Is it Viable?

Menachem Elimelech (Department of Chemical and Environmental; engineering, Yale University)

#### Abstract

In recent years, the development of nanoporous membranes has revitalized the prospect of harvesting blue energy by controlling the mixing of streams with different salinities, due to the high conductance of the nanoporous membranes. In this study, we systematically analyze the performance and identify the challenges of nanopore-based power generation (NPG) at various process scales. We begin the analysis with a single nanopore, followed by a multi-pore membrane coupon, and ending with a full-scale system. We confirm the high power densities attainable by a single nanopore, and demonstrate that at the coupon scale and above, concentration polarization severely hinders the power density of NPG, revealing the common, yet significant error in linearly extrapolating single pore performance to multi-pore membranes. By considering concentration polarization, we also importantly show that the development of advanced materials with exceptional nanopore properties provides limited enhancement of practical process performance. For a full-scale NPG membrane module, we find an inherent tradeoff between power density and thermodynamic energy efficiency, whereby achieving a high power density sacrifices the energy efficiency. Finally, we assess the net extractable energy of a full scale NPG system which mixes river water and seawater by including the energy losses from pretreatment and pumping, revealing that the NPG process — both in its current state of development and in the case of highly optimistic performance with minimized external energy losses — is not viable for power generation.

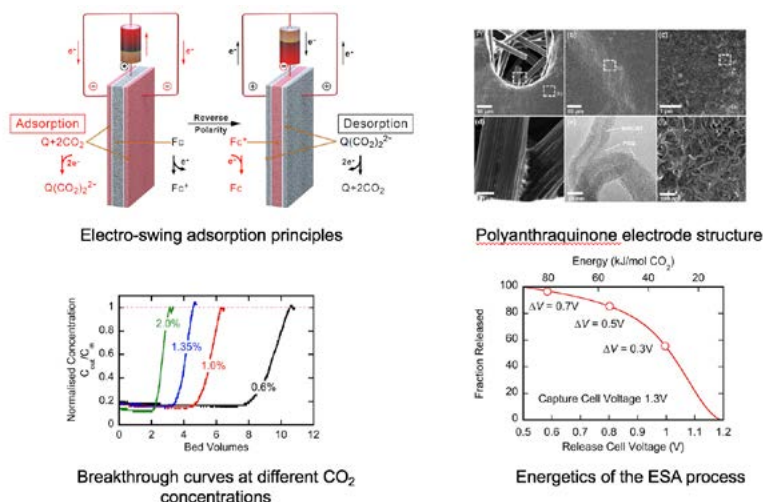


### 490 | Electrochemically Modulated Mitigation of Acid Gas Emissions

Sahag Voskian (Verdorex, Inc.), Yayuan Liu (Massachusetts Institute of Technology), T. Alan Hatton (Massachusetts Institute of Technology)

#### Abstract

Acid gas emissions pose a significant threat to the sustainability of our planet eco-system, contributing to significant global warming, changes in global climate patterns, and ocean acidification. While CO<sub>2</sub> emissions due to fossil fuel combustion are of primary concern, SO<sub>2</sub> is also increasingly being subjected to regulatory control, particularly in the maritime sector. The mitigation of these acid gas emissions is a daunting task, both because of the scale of the problem and because of the economic ramifications associated with the capture of the acid gases and their subsequent utilization, disposal or subsurface storage. Traditional acid gas capture technologies rely on chemical or physical sorption in solvents or on solids and usually require significant energy integration or large chemical inventories. We will present a versatile electro-swing adsorption technology in which immobilized redox-active complexes react with acid gases upon activation by electrochemical reduction, and release them when re-oxidized on reversal of the applied cell voltage. The adsorbents can be used in a membrane-like configuration with electrochemical gating on the feed and product sides. The principles underlying the technology, including the design and synthesis of the electroactive moieties, and the overall energetics and economics of the process, will be described.



#### Biography: T. Alan Hatton

T. Alan Hatton is the Ralph Landau professor and director of the David H. Koch School of Chemical Engineering practice at MIT, where he is also codirector of the MIT Energy Initiative Center for Carbon Capture, Utilization and Storage. His work focuses on novel technologies for addressing environmental problems in the aquatic and air environments, primarily on the use of electrochemical methods to modulate selectivity and capacity of separation processes.

### 413 | Development of photoelectrochromic windows with improved optical and electrical performance

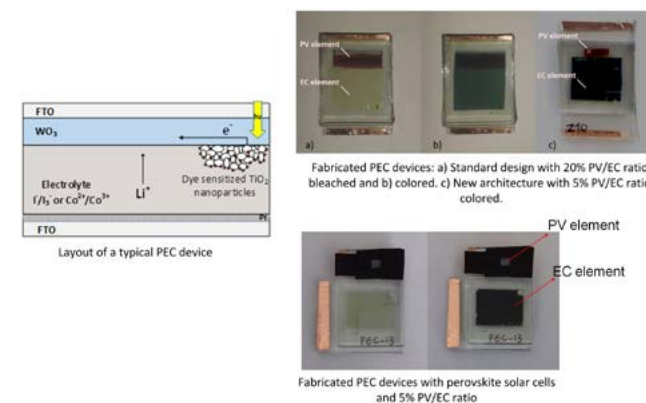
George Leftheriotis (Physics, University of Patras, GREECE), George Syrokostas (ICEHT, Patras), Alexandros Dokouzis (Physics, University of Patras, GREECE), Dimitra Zoi (Physics, University of Patras, GREECE)

#### Abstract

The integration of photovoltaics and smart windows has attracted a considerable research interest recently, due to its promising potential for simultaneous renewable energy production and energy savings. Photoelectrochromics (PECs) constitute the next generation of smart windows, combining a photovoltaic cell and the optically active electrochromic element into one device. The present work reports the use of different material combinations and device architectures aiming to improve the long-term performance of PECs. For that purpose, various electrochemical methods, such as cyclic voltammetry, electrochemical impedance spectroscopy and galvanostatic intermittent titration, were applied to investigate the processes involved in PECs: Li ion diffusion, redox reactions, electrocatalytic activity and barrier layer performance. The PEC devices thus developed exhibit favorable performance and long term durability [1,2]. Alternative architectures enabled an increase of the PV element efficiency by a factor of 4. As a result, the PV/EC area ratio has been reduced from 20% to 5%, with the coloration speed of the devices remaining unaffected. Use of perovskite solar cells instead of dye sensitized ones has also been attempted with promising results.

[1] Dokouzis A. et. al. Solar Energy Materials and Solar Cells 182(2018)281

[2] Theodosiou K. et. al. Solar Energy Materials & Solar Cells 202(2019)110124



#### Biography: George Leftheriotis

George Leftheriotis is associate professor of Renewable Energy Sources, at the Department of Physics, University of Patras. He studied Physics at the University of Patras and having received an EU grant, he carried out postgraduate studies at Warwick University, UK, receiving the MSc degree in Engineering (by research, with distinction) in 1989 and the PhD degree in 1992. His research interests include the development of materials and devices for solar energy applications, such as low-e coatings, photovoltaics and electrochromics. He has published 51 papers in refereed international journals and 81 conference contributions. He has about 1500 citations (H-index 21).

### 592 | Minimal Bipolar Membrane Cell Configuration for Scaling Up Ammonium Recovery

Mariana Rodrigues (Wetsus), Thiago de Mattos (Wetsus), Tom Sleutels (Wetsus), Annemiek ter Heijne (Wageningen University and Research), Bert Hamelers (Wetsus), Cees Buisman (Wetsus / Wageningen University & Research), Philipp Kuntke (Wetsus)

#### Abstract

Electrochemical systems for total ammonium nitrogen (TAN) recovery are a promising alternative compared with conventional nitrogenremoval technologies. To make them competitive, we propose a new minimal stackable configuration using cell pairs with only bipolar membranes and cation-exchange membranes. The tested bipolar electro dialysis (BP-ED) stack included six-cell pairs of feed and concentrate compartments. Critical operational parameters, such as current density and the ratio between applied current to nitrogen loading, were varied to investigate the performance of the system using synthetic wastewater with a high nitrogen content as an influent ( $\text{NH}_4^+ \approx 1.75 \text{ g L}^{-1}$ ). High TAN removal (>70%) was achieved for a load ratio higher than 1. At current densities of  $150 \text{ A m}^{-2}$  and load ratio of 1.2, a TAN transport rate of  $1145.1 \pm 14.1 \text{ gN m}^{-2} \text{ d}^{-1}$  and a TAN-removal efficiency of 80% were observed. As the TAN removal was almost constant at different current densities, the BP-ED stack performed at a high TAN transport rate ( $819.1 \text{ gN m}^{-2} \text{ d}^{-1}$ ) while consuming the lowest energy ( $18.3 \text{ kJ gN}^{-1}$ ) at a load ratio of 1.2 and  $100 \text{ A m}^{-2}$ . The TAN transport rate, TAN removal, and energy input achieved by the BP-ED stack demonstrated a promising cell configuration for upscaling.

#### Biography: Mariana Rodrigues

Mariana Rodrigues is a PhD student at Wetsus. Her research focus on the topic Recovery of Ammonia using electrochemical systems. She completed in 2018 the Master of Biological Engineering on the Faculty of Engineering of Porto University, Portugal.

### 557 | Electro dialysis processes for minimizing waste production in phosphoric acid plants

Lior Monat (Ben Gurion University), Oded Nir (Ben Gurion University)

#### Abstract

Fertilizers prepared from phosphoric acid are essential for meeting the increased global demand for food. However, significant amount of waste byproducts is generated in the production of phosphoric acid. The solid waste comprises of phosphogypsum ( $\text{CaSO}_4 \cdot n\text{H}_2\text{O}$ ) with residual P and trace elements. The liquid wastewater is acidic and has the potential to precipitate sparingly soluble salts. Both waste by-products are currently accumulated in piles or ponds, posing environmental and health risks. Costeffective solutions are therefore needed for increasing the sustainability of phosphoric acid production. We studied the integration of advanced electro dialysis processes as part of a physicochemical process scheme to treat the phosphoric acid wastes, while recovering valuable resources (Fig. 1). We used bipolar membranes electro dialysis as part of an overall treatment for phosphogypsum and explored the use of electro dialysis incorporating monovalent-selective cation-exchange membranes to tackle the acidic wastewater. We studied the effect of different operational parameters and quantitatively assessed the feasibility of the processes in terms of efficiency, energy consumption and operating costs, while revealing the trends, trade-offs and interrelations between the key process parameters and membrane types. Our results indicate that novel electro dialysis processes are potentially cost-effective routes for minimizing the risks posed by the phosphoric acid industry.

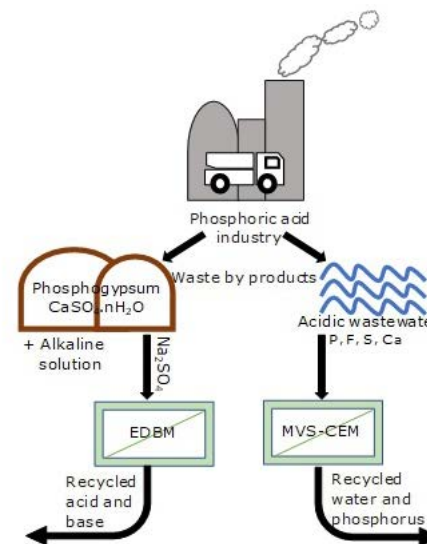


Figure 1: Electro dialysis applications to treat waste products in the phosphoric acid industry

## 598 | Harvesting CO<sub>2</sub> from the ocean for circular electrochemical carbonate mineralization

Rose Sharifian (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands), Lieneke Boer (Wetsus, European Centre of Excellence for Sustainable Water Technology, Leeuwarden, The Netherlands.), Martijn Wagterveld (Wetsus, European Centre of Excellence for Sustainable Water Technology, Leeuwarden, The Netherlands.), David Vermaas (Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands)

### Abstract

To mitigate climate change effectively, direct CO<sub>2</sub> capture from the atmosphere and ocean must be promoted. A sustainable, CO<sub>2</sub> neutral capture process can be achieved through electrochemical methods because these methods can run on renewable electricity and fit within a circular carbon economy. While the direct air capture is energy-intensive due to the low concentration of CO<sub>2</sub>(g) in the atmosphere, capturing from the ocean, which contains more than 140 times higher (dissolved) CO<sub>2</sub> concentration, is promising. We have successfully applied bipolar membrane electrodialysis to capture CO<sub>2</sub> from the seawater. Inside this electrochemical cell (Fig1), using the ability of a bipolar membrane to dissociate water, an acidic and alkaline pH are generated from the seawater feed. We present for the first time how the dissolved CO<sub>2</sub>, present as (bi)carbonates, is *in-situ* converted into valuable CaCO<sub>3</sub> and MgCO<sub>3</sub> solids via natural mineralization. Through optimization of this in-situ process (with regards to e.g., the applied current, alkaline pH, and cell design), we have achieved > 80% extraction of the oceanic dissolved inorganic carbonic species (DIC). This *in-situ* carbonate mineralization requires an electrical energy consumption of ca. 350 kJ/ mol DIC, which is 2-5 times lower than the state-of-the-art in other carbonate mineralization technologies.



### Biography: Rose Sharifian

Ir. Rezvan Sharifian is a PhD candidate in the Vermaas group, Chemical Engineering department at Delft University of technology, and concentrate theme at Wetsus, Centre of Excellence for Sustainable Water Technology, in the Netherlands. Her research focuses on new technologies for electrochemical CO<sub>2</sub> capture via pH swing. As a recipient of the full TU Delft Energy Scholarship, she graduated with her MSc with cum laude in petroleum engineering in the applied earth sciences faculty, in 2016.

## 235 | Development and upscaling of gas diffusion electrodes for wastewater treatment and electrosynthesis of chemicals

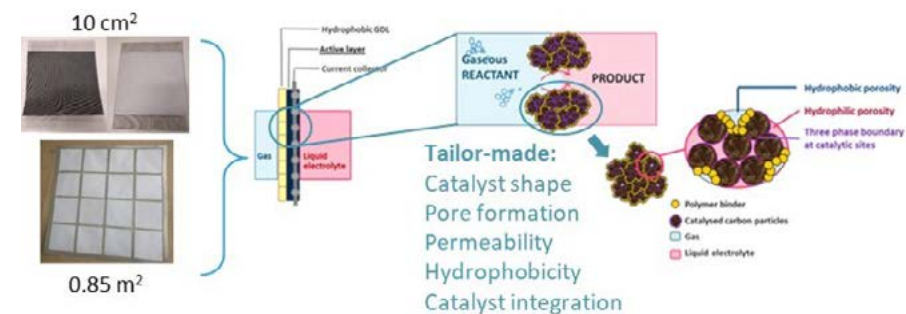
Deepak Pant (Flemish Institute for Technological Research (VITO)), Yuvraj Birdja (Flemish Institute for Technological Research (VITO)), Metin Bulut (Flemish Institute for Technological Research (VITO)), Jan Vaes (Flemish Institute for Technological Research (VITO))

### Abstract

Technologies related to gas diffusion electrodes (GDEs) offer solutions for gaseous reagents taking part in electrochemical reactions. (Bio)electrochemical processes suffer from challenges like high costs of platinized electrodes<sup>1</sup>; rapid catalyst degradation and low performance due to non-uniform electrode quality<sup>2</sup>; difficulties in upscaling. Scaling up microbial fuel cells (MFCs) requires use of large electrodes which are often difficult to fabricate without loss in quality. VITO has developed GDEs tailored for systems with aqueous electrolytes and a gas-water interface, which are characterized by controllable pore diameters in the polymer-bound active layer, mechanical robustness and low water permeability<sup>2</sup>. These cold-rolled (VITOCORE®) and phase-inversion based (VITO CASE®) electrodes enable reproducible quality in sizes from 10 cm<sup>2</sup> to 1 m<sup>2</sup>. Large-scale VITOCORE® air cathodes were recently developed and tested in 85 L and 255 L MFCs to evaluate the impact of the cathode size on MFC performance<sup>4,5</sup>. For CO<sub>2</sub> electroreduction, GDEs based on Sn, Cu and Pd were developed and evaluated for production of formic acid and oxalic acid.

### References

- [1] J. Materials Chemistry A, 7(42), 24420, 2019.
- [2] Electrochim. Acta, 82, 415, 2012.
- [3] Curr. Opin. Green Sustain. Chem., 16, 47, 2019.
- [4] Wat. Res. 148, 51, 2019.
- [5] Biores. Technol., 294, 122227, 2019.



### Biography: Deepak Pant

Dr. Deepak Pant is a Senior Scientist at the Flemish Institute for Technological Research (VITO), Belgium. His research focuses on design and optimization of bioelectrochemical systems for energy recovery from wastewater and microbial electrosynthesis for production of value-added chemicals through electrochemically driven bioprocesses. He has 5 books, 6 Patents, 138 peer-reviewed publications with >10500 citations (h-index 59) and 35 book chapters to his credit. He is a member of scientific societies like ISMET, ISE, RSC, BES, BRSI, IFIBiop and AMI. He is Editor for "Bioresource Technology Reports" and Editorial board member for 'Bioresource Technology', 'iScience', and 'ACS Sust Chem Eng'.

## 568 | Proton-mediated redox couple to enable ammonia removal and recovery

Taeyoung Kim (Clarkson University), Weikun Chen (Clarkson University), Shane Rogers (Clarkson University), Stefan Grimberg (Clarkson)

### Abstract

Domestic wastewater contains ammonia nitrogen that could potentially supply 30% of global fertilizer demand if recovered using a viable technology. One way to selectively recover ammonia from wastewater is to convert ammonium into ammonia by elevating the solution pH. However, conventional air stripping approaches limit their broader implementations due to intensive chemical and energy inputs. To circumvent this challenge, we developed a new electrochemical method to achieve simultaneous removal of ammonium and its conversion into ammonia by elevating pH, enabled by a proton-mediated redox couple (e.g.,  $R + H^+ + e^- \rightarrow O$ ). The use of redox couple allowed for energy-efficient electrochemical reactions compared to electrolysis of water in electrodialysis-based approaches. Our proof-of-concept study demonstrated that  $NH_4^+$  in a synthetic domestic wastewater (5 mM  $NH_4Cl$  + 20 mM NaCl) was separated through a cation exchange membrane at a nitrogen flux of 34 g N  $m^{-2} d^{-1}$  and 0.47 V. The solution pH was simultaneously elevated to 9.6 by the electrochemical reaction, which was sufficient to recover ammonia by membrane stripping. These results indicate that the use of a proton-mediated redox couple could represent a new strategy to enable efficient ammonia removal and recovery from wastewater.

### Biography: Taeyoung Kim

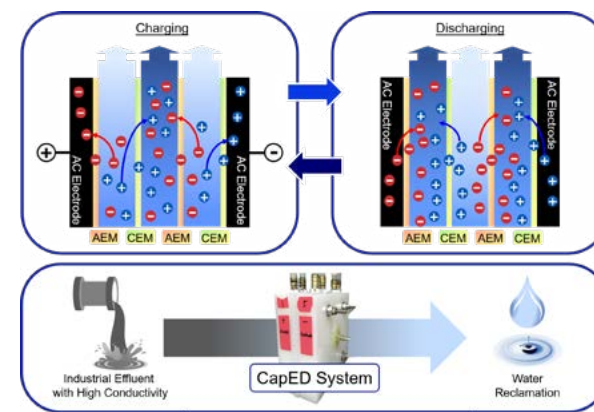
Taeyoung Kim is an assistant professor at Clarkson University with a joint appointment to the Department of Chemical and Biomolecular Engineering and Institute for a Sustainable Environment (ISE). Dr. Kim received a doctorate in the School of Chemical and Biological Engineering from Seoul National University in 2015 and was a postdoctoral scholar in the Department of Civil and Environmental Engineering at The Pennsylvania State University.

## 442 | A feasibility study of hybrid capacitive-electrodialysis deionization system for wastewater reuse in the hightech industrial park

Tsai-Hsuan Chen (National Taiwan University), Chia-Hung Hou (National Taiwan University)

### Abstract

Advanced electrochemical processes have attracted a great deal of attention to separate ions from wastewater treatments for reducing energy consumption. Electrodialysis is an electrically driven process based on ion migration of electrochemical separation. Capacitive deionization (CDI) is an electrosorption process using nanoporous carbon electrodes to store ions at a low voltage. In this study, a new membrane cell configuration for integrating capacitive electrodialysis deionization (CapED) is proposed. The CapED cell is composed of two activated carbon electrodes and three channels. The cathode and anode are covered by cation-exchange and anion-exchange membranes, respectively. Three channels are separated by anion-exchange and cation-exchange membranes. During charging/discharging, the desalinated water and concentrated water flow alternatively on either side of the membranes. Therefore, continuous deionization can be achieved by cyclic charging-discharging process. Due to contribution of both electrochemical separation and capacitive electrosorption, CapED process has a high charge efficiency. As increasing the operation voltage from 1.0 V to 2.5 V, the salt removal amount for 0.05 M NaCl solution can be enhanced from 17.53 mg-NaCl to 81.65 mg-NaCl, respectively. Furthermore, the industrial effluent with high conductivity will be tested by CapED system for the feasibility of further application in wastewater reuse from high-tech industrial park.



### Biography: Tsai-Hsuan Chen

Tsai-Hsuan Chen is a Ph.D student of Graduate Institute of Environmental Engineering at National Taiwan University. Her work focuses on electrochemical water treatment, capacitive deionization technology, and advanced nanoporous carbon materials, especially on issues that require a specialist understanding of several disciplines, and the cooperation among them. Her recent academic activities can be found in American Chemical Society, KKNN Symposium, and Mainland-Taiwan Environmental Protection Conference. She has also won several awards, such as third place of TECO Green Tech International Creative Competition and third place of Taiwan Innovation Technology Expo.

#### 494 | Q. Shu, Combined electrochemical desorption of CO<sub>2</sub> and recovery of alkaline sorbent for direct air capture

Mr. Qingdian Shu (Wetsus / Wageningen University & Research), Dr. Louis Legrand (Wetsus / Wageningen University & Research), Dr. Philipp Kuntke (Wetsus), Dr. Michele Tedesco (Wetsus, European Centre of Excellence for Sustainable Water Technology), Dr. Bert Hamelers - Wetsus

##### Abstract

Direct air capture (DAC) is widely recognized as a promising solution to reach negative emissions, and technologies using an alkaline solution as sorbent have already been demonstrated on a full scale. With the conventional temperature swing process, the subsequent desorption of CO<sub>2</sub> and the recovery of the alkaline solution is highly energy demanding. In this study, we experimentally demonstrate the simultaneous CO<sub>2</sub> desorption and solvent regeneration in a continuous system by introducing an H<sub>2</sub> recycling electrochemical system (Figure 1). Hydrogen is oxidized at the anode, and the H<sup>+</sup> produced is transported to the adjacent compartment. The resulted low pH facilitates the CO<sub>2</sub> desorption. Water reduction at the cathode produces OH<sup>-</sup> so that the alkaline sorbent is regenerated. Moreover, the generated H<sub>2</sub> compensates the gas consumption at the anode. The minimum energy consumption of the system was predicted to be 164 kJ·mol<sup>-1</sup> CO<sub>2</sub> at 25 A·m<sup>-2</sup> by a mathematical model based on chemical equilibrium and mass balance. At the same time, the NaOH solution can be recovered and reused as a sorbent for direct air capture. We have shown for the first time the use of an electrochemical cell for DAC that provides low energy requirements compared to state-of-the-art technologies.

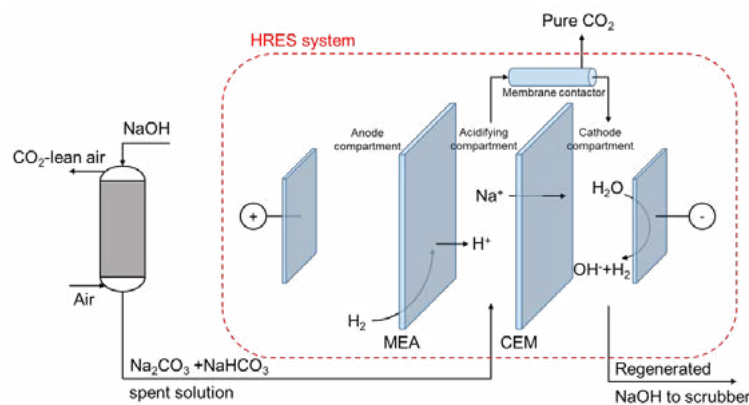


Figure 1. Principle of DAC process with H<sub>2</sub> recycling electrochemical system (HRES) for CO<sub>2</sub> desorption and regeneration of alkaline solution.

##### Biography - Qingdian Shu

Qingdian Shu is a Ph.D. candidate at Wetsus and Wageningen University. He obtained his master's degree in water technology at Wetsus Academy. He started to work on electrochemical CO<sub>2</sub> capture since his master thesis at Wetsus which was entitled 'Characterization of an innovative chemical-free CO<sub>2</sub> capture process using membrane capacitive deionization (MCDI)'. His current research focus is on electrochemical processes for direct air capture.

#### 159 | Switchable Oxygen Depolarized Cathodes in flexible Chlor-Alkali Electrolysis

Kristina Baitalow (RWTH Aachen University, Aachener Verfahrenstechnik-Chemical Process Engineering)

##### Abstract

The worldwide energy sector is facing the challenge to reduce carbon dioxide emissions, mitigate global warming, and revolutionize energy generation. With increasing proportion of renewable energy production come strong fluctuations in supplied energy. In our work, we try to reduce the energy demand of chlor-alkalielektrolysis and to adopt the processes to flexible production conditions. A new type of oxygen depolarized cathodes (ODC) can be operated flexibly while reducing the energy consumption of chlorine-alkali-electrolysis by 30 %. Bifunctional, so-called *switchable ODCs* (sODC) enable an energy-saving oxygen-consuming mode and an energy-intensive hydrogen-evolving mode. Thus, in times of large energy amounts, the oxygen mode is employed whereas in times of low energy quantities the hydrogen mode is applied.

Experiments on lab-scale focused on the system's stability for up to 1000 switching cycles and the performance of the sODC compared to a conventional ODC (no ability for switching). Stable long-term performance and a difference in cell potential between sODC and conventional ODC in a range of 5 % demonstrate the high potential of the sODC. Intensive economic studies show that introducing the sODC in chlor-alkali electrolysis can reduce operational costs by 6.5 % and accommodates the expected strong fluctuations in renewable energy sources.

##### Biography: Kristina Baitalow

Kristina Baitalow studied Mechanical Engineering at RWTH Aachen University. Currently, she works as a PhD candidate for Prof. Matthias Wessling at Chemical Process Engineering in Aachen. Her topic includes chlor-alkali electrolysis and electrochemical-cell design. To investigate flexibility in electrochemical processes, she focuses on varying load cycle experiments, CFD simulations and cell design optimization.

### 462 | Resource-efficient lithium and sodium recovery from brines using membrane electrolysis

*Luiza Bonin (Centre for Microbial Ecology and Technology (CMET), Ghent University, Coupure Links 653, B-9000 Gent, Belgium), Guillaume Henderson (Center for Microbial Ecology and Technology (CMET), Faculty of Bioscience Engineering, Ghent University, Coupure Links 653, Ghent 9000, Belgium), Victoria Flexer (Centro de Investigación y Desarrollo en Materiales Avanzados y Almacenamiento de Energía de Jujuy-CIDMEJu (CONICET-Universidad Nacional de Jujuy). Av. Martijena S/N, Palpalá, 4612, Argentina), Korneel Rabaey (Centre for Microbial Ecology and Technology (CMET), Ghent University, Coupure Links 653, B-9000 Gent, Belgium)*

#### Abstract

Selective lithium recovery from aqueous solutions is an actual demand. Unfortunately, the most common methods to extract lithium are based on huge volumes of water evaporation, high chemical usage and waste production. This work presents an integrated system to treat raw salty lake brines without evaporation. The used method combines membrane electrolysis with crystallization units is driven by electricity, with minimal input of chemicals and water. The brine was treated by ion exchange resins to extract B. The boron free brine was then sent to a crystallizer where Mg and Ca carbonates are precipitated after addition of  $\text{Na}_2\text{CO}_3$ . Brine free of bivalent ions is then added to an electrochemical cell where pH and Li concentrations are increased. The obtained alkaline brine is transferred to a crystallizer where  $\text{CO}_2$  is fluxed until pH 11 is reached, 74,4% Li is crystallized as  $\text{Li}_2\text{CO}_3$  with 96,80% purity and energy input of 79.1 kWh kg<sup>-1</sup>  $\text{Li}_2\text{CO}_3$ . The remaining solution is fluxed until achieving pH 8.5, enabling the precipitation of 28,5% Na as  $\text{NaHCO}_3$ . The obtained Na is dried at 105°C and converted to  $\text{Na}_2\text{CO}_3$  99% purity. Mg and Ca precipitation was also performed using the precipitated  $\text{Na}_2\text{CO}_3$  showing circularity of the process.

#### Biography: Luiza Bonin

Dr. Luiza Bonin is a postdoctoral research fellow at Ghent University. She is a Materials Engineer, and she obtained her PhD in Engineering Science and Technology at the University of Mons (Belgium) in 2018. Her main research focus is typically at the interface between materials, electrochemistry and environmental issues. As an example, she is currently working on the development electrochemical process for Li extraction. She has experience in electrochemical metal/resource recovery and membrane electrolysis process.

### 336 | Electrosorption using new biosourced porous electrode material for phenolic compounds removal and valorization – Electrochemical engineering aspects

*Amina Lissaneddine (Laboratoire Réactions et Génie des Procédés, Université de Lorraine, CNRS, LRGP, F-54000 Nancy, France), Emmanuel Mousset (Laboratoire Réactions et Génie des Procédés, Université de Lorraine, CNRS, LRGP, F-54000 Nancy, France), Faissal Aziz (Laboratory of Hydrobiology, Ecotoxicology, Sanitation and Climate change (LHEAC-URAC33), Faculty of Sciences Semlalia, Cadi Ayyad University, Marrakech, Morocco), Marie-Noëlle Pons (CNRS), Laila Mandi (Laboratory of Hydrobiology, Ecotoxicology, Sanitation and Climate change (LHEAC-URAC33), Faculty of Sciences Semlalia, Cadi Ayyad University, Marrakech, Morocco)*

#### Abstract

Olive mill wastewater contains a large proportion of phenolic compounds leading to high chemical oxygen demands (COD) (around 110 g-O<sub>2</sub> L<sup>-1</sup>). The saturation in aromatic molecules make difficult the treatment of such industrial effluents. Moreover, phenol and its derivatives have antioxidant and bioactive properties that could be valorized. Electrosorption technology is a separation process that has the advantages of being selective and can favor the desorption by potential control. The energy requirement can be also minimized with an adequate reactor design. In this study, a new porous material was prepared based on olive pomace activated carbon of, in the aim at valorizing the solid waste of olive oil extraction processes. This work is part the zero liquid and waste discharges approach. The electrosorption performance of this electrode was evaluated in a fixed-bed reactor operated in a cocurrent flow system. The granular activated carbon (GAC) material was connected to a potentiostat using a carbon graphite rod as current collector. The electrochemical parameters of the 3D electrode were determined (electroactive surface, electrical conductivity, mass transfer coefficient, double layer capacitance...). The electrosorption isotherms and the potential dependence of the adsorption coefficient were assessed and the matrix effect considered.

#### Biography: Amina Lissaneddine

Amina Lissaneddine is a second-year PhD student at Cadi Ayyad University (Morocco) and Lorraine University (France). She is working for 2 years in the area of adsorption and water treatment. Her supervisors (i.e. co-authors) are worldwide recognized scientists in their research fields, adsorption in Morocco and electrochemistry & chemical engineering in France, both partners focusing on environmental applications. They are particularly involved at international level in conferences organization, editorial boards in journals, boards in societies (IWA, ...), and have been awarded (one of them got the “Green electrochemistry” prize from ISE/Elsevier (2018)).

## 281 | Beneficiation of jarosite waste assisted by electrochemical operations

*François Lopicque (Université de Lorraine), Abdoulaye Maihatchi (CNRS), Marie-Noëlle PONS (CNRS), Quentin Ricoux (Extracthiv), Frederic Goettmann (Extracthiv)*

### Abstract

Jarosite is generated in zinc production processes to remove by precipitation trivalent iron species contained in the acidic liquors recovered from zinc ore leaching. Up to now the solids generated although little hazardous, are merely disposed. A hydrometallurgical pathway has been designed here to beneficiate industrial jarosite waste by preparation of valuable Fe-Zn alloys with electrochemical techniques.

Jarosite-containing wastes were first leached in sulfuric solution; concentrated Fe (III) species solutions were reduced to Fe (II) by addition of blende ore (zinc sulfide) in a second stage, with electrochemical monitoring of the reduction progress. Presence of copper in the blende resulted in undesired presence of copper ions in the solutions recovered, in addition to zinc cations. Fe-Zn alloys could then be produced by electrodeposition, but only after removal of copper ions. For this purpose, a strategy relying upon successive electrodeposition stages has been developed, with formation of first little valuable Cu-rich deposits, then high purity Fe-Zn alloys: based on a model for discontinuous deposition at fixed current density, experiments have been designed then carried out for estimation of the model parameters. The model developed can be used depending on the targeted alloy purity and recovery fractions of Fe and Zn.

### Biography: François Lopicque

François Lopicque is a CNRS research professor active in electrochemical engineering for energy conversion, as well as for waste treatment and beneficiation, within national and European projects with research centers and industry. He is a member of the working party on Electrochemical Engineering of the EFCE, and has been involved in the ISE Division "Electrochemical technology and Engineering".

## Plenary: The binomial Technology Readiness Level / Environmental Electrochemical Engineering: where are we and where are we going?

*M. Rodrigo (Universidad de Castilla-La Mancha, Spain)*

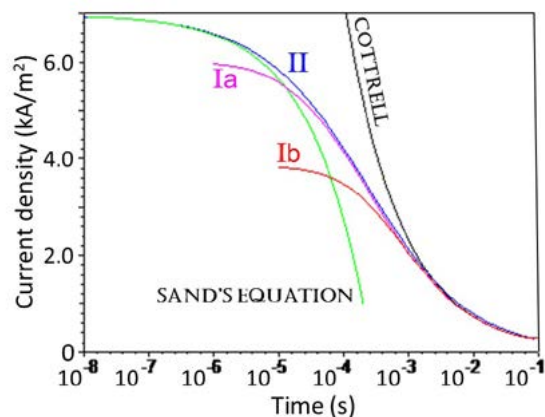
Over the last decades, electrochemical engineering is proposing alternatives for facing different environmental problems. Results obtained are diverse: promising, always; successful, sometimes. This fact indicates the necessity of additional further work for fitting the technologies into the applications. This lecture summarizes the main challenges that researchers must face in the next decade to raise the technology readiness level (TRL) of the different electrochemically-assisted environmental remediation processes, highlighting the role required for academics and companies. To do this, it is discussed the current state of the art of the environmental electrochemical technologies, based on recent experimental studies. Then, the removal of chlorinated hydrocarbons from polluted soil, the disinfection of fresh and reclaimed water, removal of anthropogenic pollutants from industrial wastes, treatment of gases by electro-scrubbing and treatment of hospital effluents are discussed as several of the most promising applications. As well, it is discussed the powering of environmental electrochemical processes using renewable energy sources, in the search of more sustainable treatments. These results help to fix the main limitations found, the points where the efforts should be concentrated to increase the TRL, and who should do this work to make these technologies more competitive and widely applied.

## 574 | The dynamics of combined ion transport and electrode reactions – Revisiting Bard, Faulkner, and Vetter

Maarten Biesheuvel (Wetsus), Jouke Dykstra (Wageningen University and Research)

### Abstract

Electrode kinetics and mass transport are coupled in realistic models in electrochemical engineering, which is doable in steady-state, but becomes much more complicated in dynamic situations, like in Faradaic processes studied in a three-electrode system by applying a step change in  $E$ , or cycling between two limiting values as we do in cyclic voltammetry. Bard and Faulkner consistently assume in this analysis that the electrode reaction is infinitely fast, which leads to the prediction of initially an infinitely high current described by the Cottrell equation. This is strange because why study an electrode reaction that is infinitely fast. Vetter takes the more realistic approach that initially, even for a very fast reaction, the reaction is 100% rate limiting. Therefore there is always a limit to the current, and Sand's equation results. We discuss these situations, and also address the role of the potentiostat, where we do not apply a step change in  $E$ , but only change a *setpoint for  $E$*  after which the potentiostat increases the current. We analyze how overshoots or oscillations are now possible. We also address the coupled process of competing electrode reactions, i.e., the topic of electrode selectivity.



### Biography: Maarten Biesheuvel

Dr. P.M. (Maarten) Biesheuvel is principal scientist at Wetsus, The Netherlands. He is a 2018 Clarivate Analytics Highly Cited Researcher and is in the Stanford Top-2% list. He has published over 100 papers in the field of electrochemical engineering, for instance about EDL theory, fuel cells, electrodialysis and capacitive deionization. He is member of the international scientific working groups on CDI&Electrosorption (2000 participants) and Physics of Membrane Processes (500 participants). With J.E. Dykstra he is author of the graduate level textbook "Physics of Electrochemical Processes" (2020). He owns a forest.

## 367 | Utilizing Polarity Reversal in Electrocoagulation to Reduce Electrode Passivation and Enhance Treatment Performance

Markus Ingelsson (Department of Chemical & Petroleum Engineering, University of Calgary), Behzad Fuladpanjeh Hojaghan (Department of Chemical & Petroleum Engineering, University of Calgary), H line Chow (Department of Civil & Environmental Engineering, University of Waterloo), Milana Trifkovic (Department of Chemical & Petroleum Engineering, University of Calgary), Anh Pham (Department of Civil & Environmental Engineering, University of Waterloo), Edward Roberts (Department of Chemical & Petroleum Engineering, University of Calgary)

### Abstract

In water treatment, electrocoagulation (EC) has been identified as a potentially more sustainable method than traditional chemical coagulation. EC does not require addition of metal salts and pH-neutralizing chemicals. Instead, the addition of coagulant occurs in-situ by the electrochemical dissolution of the anode combined with hydroxide formation at the cathode. However, material precipitation on the electrodes can create operational problems. To address this, periodically reversing electrode polarity has been proposed. In this study, bench scale EC reactors were used to determine the dissolution efficiency using iron and aluminum electrodes at different polarity reversal frequencies and water compositions. Fouling was quantified by dissolving the electrode surface layer in acid, followed by ICP-OES analysis. Chronopotentiometry and voltammetry were conducted to identify the electrochemical reactions at the electrodes. The current efficiency was dependent on the reversal frequency and the water composition for both iron and aluminum electrodes. For iron, fast reversal increased electrode fouling and inhibited coagulant production. Side reactions and changes in pH at the electrode interfaces were hypothesized to cause this effect. However, longer reversal periods improved the overall process performance. Aluminum electrodes did not exhibit the same sensitivity to side reactions, but fouling was still high in polluted waters.

### Biography: Markus Ingelsson

Markus joined the University of Calgary as an M.Sc. chemical engineering student in 2019 after graduating cum laude from the University of Vermont with a B.Sc. in Environmental Engineering. As an undergraduate student, he conducted vehicle emissions research related to the advancement of biofuels. With a great passion for developing environmentally sustainable technology, he is currently researching electrochemical water treatment systems. More specifically, understanding and enhancing the performance of electrocoagulation and electrooxidation processes for a wide range of different applications.



#### 478 | On the behaviour of low-cost MFC: The Contribution of Porous Support Materials

*Jesus Rodriguez (Centro Nacional del Hidrógeno, Puertollano (Ciudad Real)), Simonetta Palmas (cag), Laura Mais (Università degli Studi di Cagliari), Roberto Campana (Centro Nacional del Hidrógeno, Puertollano (Ciudad Real)), Michele Mascia (Università degli Studi di Cagliari), Annalisa Vacca (Università degli Studi di Cagliari), Elisa Casula (Università degli Studi di Cagliari)*

##### Abstract

Microbial fuel cells represent an emerging technology that opens the doors to different applications such as the direct production of electricity from the transformation of organic waste, or the microbial electrolysis, microbial desalination and microbial electrosynthesis.

Planning efficient and sustainable MFC systems is strictly connected, from one hand, to the deep understanding of the electroactivity of the biofilm, and from the other hand, to the use of green and economic materials for electrodes and membranes, which, at the moment, represent the main costs.

The present work investigates on the behaviour of low-cost MFC in which i) carbon-based materials are used as support for both the electrodes, ii) copper-oxide based catalyst is used instead of platinum at the cathode, and iii) ceramic membrane is used instead of Nafion.

The charge transfer mechanism occurring at the anodic biofilm is investigated and the performances of the MFC are evaluated when different carbon supports are used as cathodic materials. The favourable comparison of the results obtained, with analogous data reported in literature, is encouraging for future developments in this direction.

#### 471 | Modelling ion transfer through ion exchange membranes in electro dialysis for multi-ionic solutions

*Selin Özkul (Wageningen University and Research), Jonathan van Daal (Wageningen University and Research), Roel Bisselink (Wageningen Food and Biobased Research), Norbert Kuipers (Wageningen Food and Biobased Research), Harry Bruning (Wageningen University and Research), Jouke Dykstra (Wageningen University and Research), Huub Rijnaarts (Wageningen University and Research)*

##### Abstract

Water reuse is one of the solutions to prevent depletion of freshwater resources; however, it is often limited by accumulation of specific ions in water. Developing ion-selective desalination technologies could in many cases increase the potential for water reuse. Electrodialysis (ED) is an electrically driven membrane process in which ion transport takes place as a result of electromigration and diffusion across the membranes. Understanding these mechanisms is important to enhance the ion selectivity of the process. In this research we aim to explain these mechanisms based on theoretical and experimental studies considering multi-ionic solutions. For that purpose, a two-dimensional theoretical model was developed in order to describe the transport of ions and water through membranes in an ED cell. The computational domain of this model is a repeating unit of an ED cell, which includes one diluate channel, one cation exchange membrane, one concentrate channel and one anion exchange membrane. The two-dimensional process model describes transport of ions across the membranes with the extended Nernst-Planck equation. In order to validate the model desalination experiments were performed using a batch-mode ED setup. The effect of various operational parameters on selectivity was studied, such as the current density and the water flowrate.

##### Biography: Selin Özkul

PhD Researcher at the Department of Environmental Technology - Wageningen University and Research, the Netherlands

## 285 | Development of jet electro-absorbers for the treatment of organochlorinated wastes

Martín Muñoz Morales (University of Castilla-La Mancha), Manuel A. Rodrigo (University of Castilla-La Mancha), Cristina Sáez (University of Castilla-La Mancha), Pablo Cañizares (University of Castilla-La Mancha)

### Abstract

The treatment of gaseous pollutants using the absorption process has been applied since seventies to remove odor and harmful gases. Among the technologies developed, scrubbing is a well-known process to treat gaseous wastes used successfully to remove a simultaneous mixing of NO<sub>x</sub>, SO<sub>x</sub> and carbon dioxide. These successful results enhance the applications of scrubber for the treatment of dangerous volatile compounds that appears in the wastewater treatment plants.

However, it is necessary to improve some key factors in the design of scrubbers as the size of systems and the mass transference to avoid the high investment costs associated. Recently, a jet aerator based on the venturi effect was studied to absorb gaseous pollutants in the absence of a compressor, but higher tanks are needed for increasing the contact time to absorb gaseous pollutants in liquids.

In this work, it is described and tested an electroscrubbing system that combines the process of absorption of gaseous pollutants into a liquid stream (which acts simultaneously as absorbent and electrolyte) with electrolysis, taking advantage the low energy requirements of the jetmixers to transfer the pollutant into the electrolyte-absorbent and the powerful radical generated during the electrolysis with BDD anodes.

### Biography: Martín Muñoz Morales

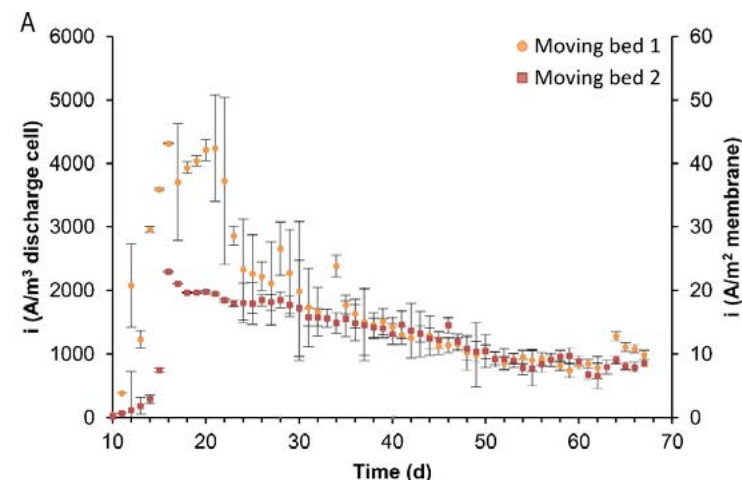
Posgraduated in the University of Castilla la Mancha in 2016 both awarded with the extraordinary mention. I started my PhD in Ciudad Real (2016) and I recently became an Associated professor at Superior Agronomic School (Albacete-UCLM). I am co-autor at the time of 18 research papers developed during the PhD and my results have been presented in more than 15 international congresses. I will finish my PhD by April, 2021.

## 102 | The granular capacitive moving bed reactor for the scale up of bioanodes

Casper Borsje (Wetsus / Wageningen University & Research), Tom Sleutel (Wetsus), Michel Saakes (Wetsus), Cees Buisman (Wetsus / Wageningen University & Research), Annemiek ter Heijne (Wageningen University and Research)

### Abstract

Bioelectrochemical systems face scaling up challenges in material costs, the limited conductivity, and clogging involved with real wastewater. The granular capacitive moving bed reactor offers possible solutions to these problems. Granular activated carbon granules are used as bioanode material while simultaneously functioning as capacitive charge storage. The charge storage abilities allow for physical separation of charging, via oxidation of organics, and discharging, at the current collector. We studied the performance of the granular capacitive moving bed reactor and compared these to a fixed bed reactor and to abiotic granules. The moving bed produced a current of 43 A/m<sup>2</sup>, about 2 times the fixed bed current density. The relatively short discharge time and long charging time of the moving bed as compared to the fixed bed bioanodes led to higher capacitive currents. Abiotic tests showed the electrical resistance was more important in determining the transferred charge than the ionic resistance. Further analysis of the resistance during discharging with different  $\Delta E$  showed discharging itself improved the discharging by local increasing conductivity. The results show the produced current is promising for further scaling up of bioanodes, though the challenge remains to improve the discharge of the charged granules.



### Biography: Casper Borsje

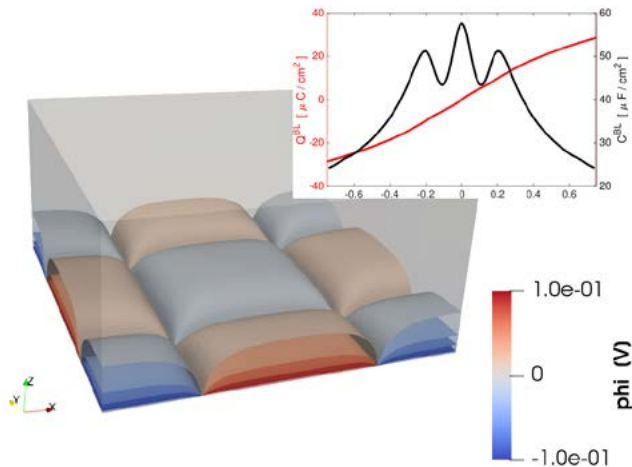
Casper Borsje is a PhD student at the department of Environmental Technology of Wageningen University, conducting his current scientific studies at Wetsus, European Centre of Excellence for Sustainable Water Technology. He obtained MSc degree in Environmental Technology at Wageningen University in 2015. He is currently working on granular capacitive bioanodes for scaling up bioelectrochemical systems, where a physical separation of oxidation of organics and harvesting of the electrical current is facilitated by charge storage characteristics of granular activated carbon.

**453 | Modeling electrode-electrolyte interfaces: The differential capacitance of polycrystalline surfaces and non-constant susceptibility**

Rüdiger Müller (Weierstrass Institute), Jürgen Fuhrmann (Weierstrass Institute), Manuel Landstorfer (Weierstrass Institute)

**Abstract**

We present and analyze a model for polycrystalline electrode surfaces based on an improved continuum model that takes finite ion size and solvation into account and allows the susceptibility to depend on the electrolyte concentration and the electric field. Numerical simulation of finite size facet patterns shows that for large facets, an ensemble of non-interacting single crystal surfaces is approached. Already for moderate facet diameters, the capacitance is remarkably well approximated by the classical approach of adding the single crystal capacities of the contributing facets weighted by their respective surface fraction. As a consequence, the potential of zero charge is not necessarily attained at a local minimum of capacitance, but might be located at a local maximum instead. We find that in the large facets limit the influence of the actual geometry of the facet pattern is negligible and our theory opens the way to a stochastic description of complex real polycrystalline surfaces. This enables the extension of the results to electrodes assembled from nano-particles. Thermodynamically consistent modeling of nonconstant susceptibility requires non-obvious changes in the system of equations. It considerably supports the modeling efforts to limit the differential capacitance maxima.



**Biography: Rüdiger Müller**

Rüdiger Müller received his PhD in numerical mathematics in 1997 at Otto-von Guericke Universität Magdeburg. As a postdoctoral researcher at Humboldt-Universität Berlin, he was concerned with numerical analysis of phase field methods. Since 2009 he is researcher at Weierstrass Institut in Berlin and since 2013 he focuses on modeling a numerical simulation of electrochemical systems, thermodynamically consistent electrolyte models, transport through nanopores and characterization of heterogeneous systems.

**170 | Electrochemical Treatment of Spent Wire Drawing Solutions**

Henry Bergmann (Anhalt University, Köthen)

**Abstract**

Effective heavy metal recovery from lubricants and chemical coating solutions is a problem worldwide. In the given case,  $\text{Cu}^{2+}$  ions had to be separated from spent solutions, which were used in wire drawing and chemical copper coating on iron wires. The aim was to remove copper within limits finally allowing discharge of treated mixed wastewater to a river. The spent solutions contained mainly  $\text{H}_2\text{SO}_4$ ,  $\text{Cu}^{2+}$ ,  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  ions at a  $\text{g}/\text{dm}^3$  concentration range. Results from experiments using parallel plate electrode cells did show that copper removal is possible until ca.  $1 \text{ g}/\text{dm}^3$ . Dendritic powder formation was observed when depletion was proceeded to lower copper concentrations. As conclusion from all preliminary experiments, a decision was made to develop a 2-step technology for copper removal (Fig. 1) - consisting of a first cell equipped with special plate and extended mesh electrodes, and a second cell, the so-called Vertically Moving Particle Bed Reactor [1] able to work until a current load of  $200 \text{ A}$  and reducing copper concentration down to  $\text{mg dm}^{-3}$  concentration. This technology was successfully transferred into practice.

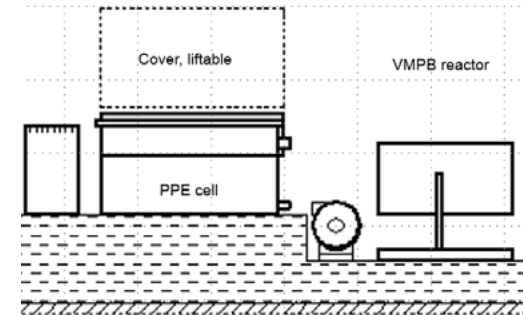


Fig. 1 The 2-cell technology developed for industrial application.

**References**

[1] Hertwig, K. et al., European Patent EP 0566907 B1.

**Biography: Henry Bergmann**

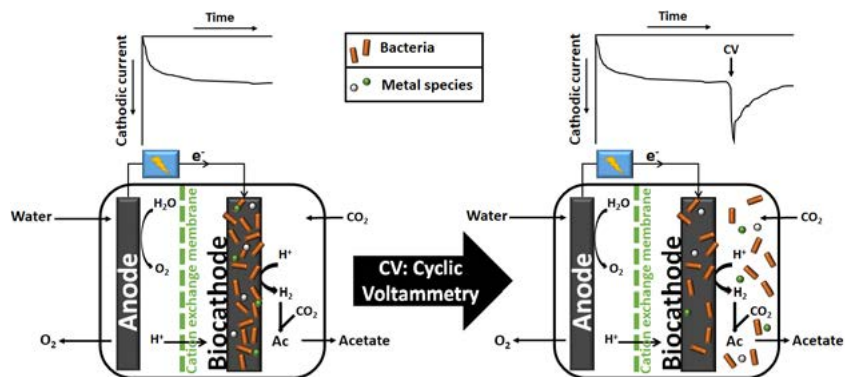
Henry Bergmann got his diploma degree from the Moscow Chemical Technological Institute D.I. Mendeleev, and PhD from the Engineering University of Koethen. Presently, he works at a professor of Anhalt University and as a director of the Institute of Environmental and Energy Technologies. In the field of Applied Electrochemistry, he is active for 40 years. Henry Bergmann is author and coauthor of more than 300 publications, posters and conference papers. Current activities are focused on new electrochemical disinfection technologies.

## 26 | Boosting a biocathode by analysis: the invasive effects of cyclic voltammetry on microbial electrosynthesis

Sanne de Smit (Wageningen University and Research), David Strik (Wageningen University and Research), Harry Bitter (Wageningen University and Research), Cees Buisman (Wetsus / Wageningen University & Research)

### Abstract

In this study, we investigated the effect of the considered non-invasive cyclic voltammetry (CV) on microbial electrosynthesis. CV repetitively enhanced current density for up to 20 days in a bioelectrochemical CO<sub>2</sub> elongation system with a developed biofilm, while the current decreased in similar abiotic systems. The concentrations of Fe, Co, Al, Ba, Mn, Mo and biomass increased in the biotic catholyte predominantly during the oxidation peak of the first CV cycle, indicating these compounds were released from the cathode. A smaller increase of Fe, Ni and Co was measured in abiotic experiments. The catholyte metal concentrations decreased rapidly within four hours after the CV at the cathodic operation potential of -0.85 V vs SHE. The oxidation peak of the first cycle of the CV had a less negative potential compared to the oxidation peaks of the second and third cycle for the biotic experiment. The results from this study support the hypothesis that the biocathode changes irreversibly during CV. These findings are potential applicable to modify or provide in-situ maintenance on biocathodes. Moreover, our findings form a starting point for follow up studies investigating the mechanisms behind the possible catalytic effects of the performed analysis method.



### Biography: Sanne de Smit

Sanne de Smit did a bachelor Life Science and Technology at the University of Delft and the Leiden University. Her enthusiasm about the application of biotechnology for solving environmental challenges led her to the Wageningen University, where she followed the master Biotechnology with the specialization environmental and biobased technology. During her master thesis she worked on methanol based chain elongation in mixed culture reactors. After finishing her master, she started a PhD on bioelectrochemical chain elongation, where she is working on the elongation of CO<sub>2</sub> to fatty acids in mixed culture biocathodic systems since September 2018.

## 339 | Proton transport across anion exchange membranes in electrochemical systems

Jouke Dykstra (Wageningen University and Research), Maarten Biesheuvel (Wetsus)

### Abstract

In many electrochemical systems amphoteric ions are present, which undergo acid-base reactions. We present theory for an electrochemical cell that includes electrochemical reactions at the electrodes and ion transport across the membranes to study the transport of the most prominent anions and cations, in combination with acid-base reactions. We analyze the transport of several amphoteric ions in two frequently used membranes in an electrochemical system: an anion exchange membrane (AEM) and a bipolar membrane (BPM). We show results for a system in which acetate (Ac<sup>-</sup>), acetic acid (HAc), bisulphate (HSO<sub>4</sub><sup>-</sup>) and sulphate (SO<sub>4</sub><sup>2-</sup>) ions are present. We find that, across the membrane, the ionic current is mainly carried by the group of ionic species with the pK<sub>a</sub> value closest to the local pH. Furthermore, we observe a net transport of protons across the AEM from the anode to the cathode, which are shuttled by the SO<sub>4</sub><sup>2-</sup> ↔ HSO<sub>4</sub><sup>-</sup> group and the Ac<sup>-</sup> ↔ HAc group. To quantify this phenomenon, we can define a 'proton shuttle number' (PSN), which is the contribution of each of these groups to proton transport.

### Biography: Jouke Dykstra

Assistant professor *electro-interfacial phenomena in water technology*  
Environmental Technology, Wageningen University, The Netherlands

Secretary of the International working group on Capacitive Deionization and Electrosorption (<http://www.cdi-electrosorption.org>)

### Scientific interests

- Electrochemical engineering, with a focus on ion separation processes
- Ion and electron transport in porous media, including membranes and electrodes
- Interfacial phenomena in (nano)porous materials (electrical double layer formation, chemical interactions, and faradaic reactions)

### Technological interests

- Capacitive Deionization for water desalination
- Electrodialysis for ion-selective separations
- Electrochemical technologies for the recovery (or up-concentration) of valuable chemicals and nutrients

## 121 | Electrochemical treatment of membrane concentrates

*Karel Denk (University of Chemistry and Technology, Prague, Dep. of Inorganic Technology), Adam Giurg (University of Chemistry and Technology, Prague, Dep. of Inorganic Technology), Martin Paidar (University of Chemistry and Technology, Prague, Dep. of Inorganic Technology)*

### Abstract

Membrane processes are a well-established way of water processing. They are a reliable source of clean water or means of waste-water treatment. In the latter case, the concentrate stream represents a challenge for subsequent treatment because of persistent organic compounds or heavy metal ions which can be present. Because of high concentrations of ionic species, these types of solutions have high conductivity and thus are suitable for electrochemical treatment.

Cathodic reduction can be used to deplete the solution of heavy metal ions such as copper, silver, nickel, etc., which can be utilized by further processing. Carbon-based electrodes are suitable for this process, as they are inexpensive and the reduced metal can be obtained by burning the electrode.

Anodic oxidation is a way of organic pollutants removing or converting to a biologically processable form. As an advanced oxidation process, it utilizes oxidizing agents (hydroxyl radicals, ozone, ...) which can be electrochemically generated from water without or with addition of a small amount of additional chemicals.

The aim of this work is to explore the possibilities of these two approaches for their future combination.

### Acknowledgements

Project No. TJ02000116 is solved with financial support of the Technological Agency of the Czech Republic.

### Biography: Karel Denk

The author is in his second year of Ph.D. studies in the University of Chemistry and Technology in Prague, Department of Inorganic Technology.

During his studies, the author focused on several research topics, mainly alkaline water electrolysis and process-water treatment. Apart from the experimental techniques, the author works with 3D-printing and laser-cutting, both of which he actively uses for the construction of experimental cells.

## 600 | Technology development of water electrolyser design in applied & fundamental domain

*Ipshita Banerjee (SHELL), Cor vanKruijsdijk (SHELL), Satya Srinivas (SHELL), Tafizur Rehman (SHELL), Vishal Ahuja (SHELL), Sridevi Govindarajan (SHELL)*

### Abstract

Hydrogen is an enabler for the energy transition and decarbonisation of transport and some other industrial processes. There is significant drive to speed up the transition by being able to make green H<sub>2</sub> cost competitive with H<sub>2</sub> from SMR. In order to do this tech development, it is required for technology development of water electrolyser to increase current density and cell durability & lower cost. Shell New Energies Research and Technology covers the full range of research from fundamental investigations into new components and designs, through to technology upscaling, piloting and deployment support. In the fundamental research program, the focus is on study of cell design & architecture (CD&A) of different electrolyser design, and research on alkaline exchange membrane (AEM). Electrochemical Microscopy Lab works with Water Electrolyser program for hydrogen synthesis providing state of the art research activities to support Shell through energy transition journey. AFM imaging of various electrocatalyst morphologies, quantification of their roughness and analysing the trends with respect to other performance factors like electrochemical activity will be reported. Study of nucleation, growth, attachment of nanobubbles produced at electrode/electrolyte interface in electrochemical systems and their effect on efficiency and performance of the electrolyser will also be discussed.

### Biography: Ipshita Banerjee

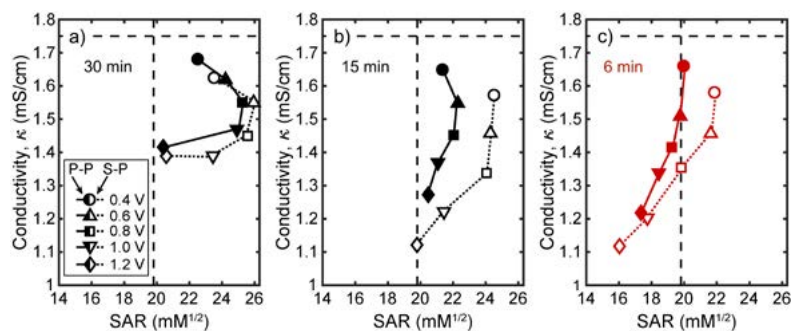
Ipshita Banerjee holds a PhD in Chemical Engineering with focus on Nanotechnology & Material science engineering, from Indian Institute of Science, Bangalore. Dr. Banerjee primarily supports the Water Electrolyser R&D program in Shell to produce hydrogen and build up an integrated computational / experimental program to study fundamentals of water-splitting reaction both in macro- and micro-/nanoscale domain. Prior to Shell, Ipshita worked with SABIC Technology Centre, Bangalore as Research Scientist & worked both in experimental and process simulation domain.

## 88 | Long-lasting, monovalent-selective capacitive deionization electrodes

Eric N. Guyes (Faculty of Mechanical Engineering, Technion – Israel Institute of Technology, Haifa, Israel), Amit N. Shocron (Faculty of Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel), Yinke Chen (Grand Technion Energy Program, Technion - Israel Institute of Technology, Haifa, Israel), Charles E. Diesendruck (Schulich Faculty of Chemistry, Technion – Israel Institute of Technology, Haifa, Israel), Matthew Suss (Faculty of Mechanical Engineering, Technion - Israel Institute of Technology, Haifa, Israel)

### Abstract

Ion-ion selectivity, the preferential removal of particular charged species in a competitive ionic environment, is an active and growing research topic in capacitive deionization (CDI). We here study monovalent selectivity, the preferential removal of a monovalent ion in the presence of a divalent ion, with the aim of reducing the sodium adsorption ratio (SAR) of a test feed stream for agriculture irrigation. Using a flow-through electrodes CDI cell operated in constant-voltage mode, we characterize the selectivity performance of a pristine cathode (P-P cell) and a functionalized cathode containing sulfonic groups (S-P cell) for a feed water containing  $\text{Na}^+$  and  $\text{Ca}^{2+}$  ions for full cycle times (FCT) 6–30 min and voltages 0.4–1.2 V. At longer FCT, both cathode types raised SAR above the feed value (panels a,b), possibly causing soil infiltration issues. However, at FCT 6 min and 1.2 V, the S-P cell reduced SAR to 16, improving water quality relative to the feed (panel c). The lower output SAR from the S-P cell is due to greater selective removal of  $\text{Na}^+$ , which is exhibited over 1000 charge-discharge cycles with a highest achieved  $\text{Na}^+$  separation factor of 1.6, indicating the promise of functionalized materials for enhanced, long-lasting monovalent selectivity.



### Biography: Eric N. Guyes

I was born between the gentle rolling slopes of the Appalachian Mountains in Virginia, in the southeastern United States. For undergraduate studies I attended Middle Tennessee State University, located in a city quite unlike Leeuwarden except in regard to its utterly flat terrain. There I began pilot training, but switched to a physics curriculum when I became more interested in the scientific aspects of flight than the flying itself. In 2013, I moved to Israel on a Fulbright Fellowship awarded by the U.S. State Department. Afterward, I joined Prof. Suss' lab as an M.Sc. student, eventually continuing to Ph.D. studies.

## 680 | Understanding and influencing biological conversions with electrodes

A. ter Heijne (Wageningen University, the Netherlands)

### Abstract

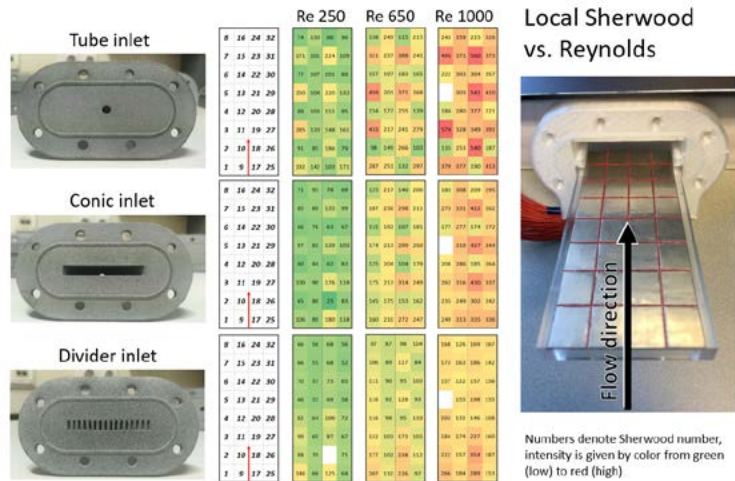
Biotechnological processes are widely applied in wastewater and gas treatment for removal and recovery of organic material, nitrogen, phosphate and sulphur. Each process has its own optimal range of Oxidation Reduction Potential (ORP). Electrodes are a unique tool to study and control microbial conversions since they can be tuned to specific potentials and in this way accept electrons from, or donate electrons to, microbial communities. The interaction between electrodes and biofilms forms the basis of Microbial Electrochemical Technologies (METs). These so-called electro-active biofilms can not only convert chemical energy into electrical energy and vice versa, but they can also store charge, for example when operated under intermittent potential control. In combination with use of capacitive electrode materials, we developed new reactor designs to continuously harvest electricity from organic matter. In addition to interaction between biofilms and electrodes, there can also be interactions between suspended bacteria and electrodes. For example, we observed that sulphide oxidizing bacteria can shuttle electrons between sulphide and the electrode, leading both to new types of applications for METs and new types of reactors. Finally, supplying microorganisms with electricity on biocathodes is a new strategy to degrade harmful components like organosulfur compounds.

### 420 | Improved reactor design using 3D printed electrolyzers

Stephane Weusten (Eindhoven University of Technology), Luc Murrer (Eindhoven University of Technology), Mattheus de Groot (Eindhoven University of Technology), John van der Schaaf (Eindhoven University of Technology)

**Abstract**

With the advent of additive manufacturing as a consumer technology, it is now possible to create highly customized components at a very small cost. In our work, 3D printing was used for quickly creating a variety of electrolyzer prototypes. Using these prototypes, different design choices could be evaluated for their effect on performance. As a first step, we focused on the rate of mass transfer as a performance indicator. In this step, the effect of the inlet design, the entrance length and turbulence promoters were investigated. Furthermore, the electrode was split into 32 independently operated segments in order to view these effects on a local scale. Depending on the configuration, differences in performance could be observed as large as an order of magnitude. For the inlet design alone, up to a factor 2.3 difference was found between the different designs. Additionally, large local variations could be observed (see attached figure). As the second step, we built an alkaline water electrolyzer using an off-the-shelf fused filament fabrication printer. The aim of this reactor is to serve as a platform for investigating intensified water splitting at process conditions up to 70°C, 1 atm and containing 30% KOH.



**Biography: Stephane Weusten**

Stephane Weusten is a 3rd year PhD candidate within the department of chemical engineering of the TU/e. His work focuses on the intensification of electrochemical reactors. As part of this work, he delved into 3D printing as a tool for creating better reactors. Initially, the goal was to intensify the chlor-alkali process, but recently the focus has shifted somewhat to water electrolysis. Currently, he is investigating a high current density electrolyzer that channels 600A to its 150cm<sup>2</sup> electrodes. He is also involved in various teaching activities, thereby transferring the know-how behind his printed electrolyzers to future researchers.

### 609 | Understanding pH changes during long-term operation of Membrane Capacitive Deionization (MCDI)

Antony Cyril Arulrajan (Wetsus / Wageningen University & Research), Jouke Dykstra (Wageningen University and Research), Albert van der Wal (Wageningen University and Research), Slawomir Porada (Wetsus, European Centre of Excellence for Sustainable Water Technology)

**Abstract**

Membrane Capacitive Deionization (MCDI) is a water desalination technology employing porous electrodes and ion exchange membranes. During the operation of MCDI, pH of the effluent water changes, which can result in scaling, affect the electrode and membrane performance. Most studies on pH changes are conducted with pristine electrodes, which are only used for a limited number of cycles. Many of these studies concluded that faradaic processes explain the observed pH changes. However, after many cycles of operation, as the electrodes age over time, the magnitude and cause of faradaic reactions can be different. In addition, non-faradaic phenomena, such as differences in transport rate of various ionic species can also cause pH changes. In our study, we used aged electrodes, and studied pH changes in a cell running on a sodium chloride feed solution, and on a more complex brackish water solution. We compared the experimentally observed pH changes with theory, which includes both faradaic and non-faradaic processes. The theory describes the experimentally observed pH changes well by only considering non-faradaic processes. The excellent agreement between the theoretical description and the experimentally observed pH changes shows the significance of non-faradaic processes on effluent pH changes during long-term operation of MCDI.

**Biography: Antony Cyril Arulrajan**

Antony Cyril Arulrajan is a Ph.D candidate at Wetsus and Wageningen University and Research, where he is doing his research in water desalination using a technology called capacitive deionization (CDI). His research is focused on understanding pH changes during CDI operation, and selective removal of ions using CDI. Antony finished his master degree in chemistry in his home country India and have research experience in material chemistry and electrochemistry.

### 599 | Modelling of a Single Chamber Bio-Electrochemical Cell for Wastewater Treatment and Clean Energy Production

Elisa Casula (Università degli Studi di Cagliari), Daniele Molognoni (LEITAT Technological Center), Eduard Borràs (LEITAT Technological Center), Michele Mascia (Università degli Studi di Cagliari), Laura Mais (Università degli Studi di Cagliari)

#### Abstract

Current treatment technologies for water pollution remediation are energy-intensive and cost consuming. A sustainable alternative is represented by Bio-Electrochemical Systems (BES), allowing the degradation of organic compounds at low energy demand with simultaneous energy and/or resources recovery from water, due to the activity of electroactive bacteria. BES performance is affected by several parameters. A three-dimensional mathematical model is presented here to support optimization of the BES performance in terms of electrical current generation and substrate/pollutant removal. The model accounts for system fluid-dynamics, material transport, (bio)electrochemical reactions, and electrical charge conservation. Following a calibration through comparison with targeted experimental data, the model was used to investigate how BES performances were conditioned by selected operational parameters. Model solution obtained with the COMSOL® Multiphysics software provides time and space distribution of potential and current, substrate, protons and microorganisms concentration, and biofilm thickness, under fed-batch or flow operation. The model developed is relevant to simulate process performance under different BES applications. It will serve as prediction tool for simulating wastewater treatment, pollutants removals and potential energy harvesting

#### Acknowledgements

This work is part of a project that has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 826312

#### Biography: Michele Mascia

Chemical Engineering, Full Professor of Chemical Plant design at the Department of Mechanical Chemical and Materials Engineering of the University of Cagliari. Michele Mascia has wide experience in modelling of electrochemical, photoelectrochemical and bioelectrochemical systems for environmental remediation and energy conversion. The activity focuses on catalytic activity of electrode materials and on identification of reaction mechanisms, as well as practical aspects of design and characterization of reactors. The results of all the researches have been published in international scientific journals and presented at major international conferences. Michele Mascia has been involved in several regional national and European research projects.

### 207 | Solid electrolyte based photoelectrochemical cells for solar hydrogen production

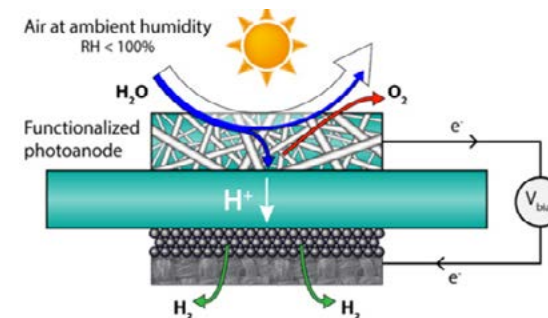
Georgios Zafeiropoulos (Dutch Institute For Fundamental Energy Research), Purushothaman Varadhan (Dutch Institute For Fundamental Energy Research), Lars Kamphuis (Dutch Institute For Fundamental Energy Research), Hannah Johnson (Toyota Motor Europe), Sachin Kinge (Toyota Motor Europe), Richard van de Sanden (Dutch Institute For Fundamental Energy Research), Michail Tsampas (Dutch Institute For Fundamental Energy Research)

#### Abstract

Due to the current climate crisis caused primarily by anthropogenic CO<sub>2</sub> emissions, there is an urgent need for alternative, green energy carriers. One such alternative is renewable hydrogen - an energy carrier which can be produced from sunlight-induced 'water splitting'- the photoelectrochemical (PEC) dissociation of water on the surface of semiconductors under irradiation<sup>1</sup>. Most of the research on PEC-reactors has focussed on using liquid water as feedstock. However, using water vapour, present as ambient humidity, can provide an interesting alternative since it enables the use of solid state devices<sup>2</sup> which are compact and scalable. These reactors, so-called polymeric electrolytic membrane PEC cells (PEM-PEC) require porous photoelectrodes for gas-flow rather than the conventional planar design used in the liquid phase. So far, this concept has been demonstrated with TiO<sub>2</sub> and WO<sub>3</sub> photoelectrodes, however due to their high band-gap, the solar-to-hydrogen-efficiency of such devices has been limited. In this study, the photoelectrode material has been expanded to BiVO<sub>4</sub>-a small bandgap semiconductor, which on porous substrates exhibits three times higher performance in the PEM-PEC cell compared to TiO<sub>2</sub> and WO<sub>3</sub>.

#### References

- [1] G. Zafeiropoulos et al, Sol. Energ. Mat. Sol. C.,180 (2018) 1  
[2] G. Zafeiropoulos et al, ACS Appl. Mater. Inter.,11 (2019) 41267



#### Biography: Michail Tsampas

Dr. M.N. Tsampas since 2014 is group leader of Catalytic and Electrochemical Processes for Energy applications (CEPEA) at Dutch Institute For Fundamental Energy Research (DIFFER). His current research is focused on energy transition with focus on renewable energy storage in chemical bonds i.e. solar fuels. A main research line of CEPEA is water splitting in photoelectrochemical cells utilizing novel operation modes and cell architectures. His research output consists of 43 journal publications (and >10 conference proceedings), one book chapter contribution and one international patent. His h-index is 17 and his work is cited >800 times (GoogleScholar Jan 2020).

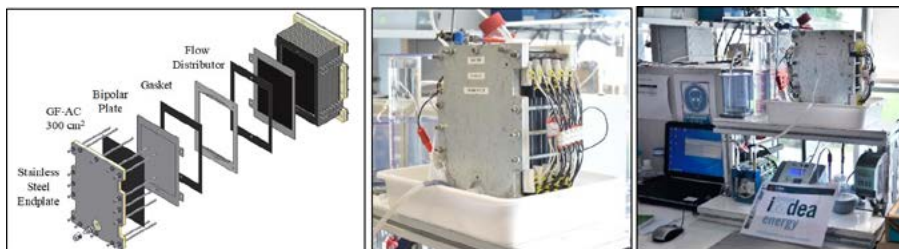


## 276 | Performance Analysis of a Capacitive Deionization Stack Equipped with Graphite Felt 3D Composites Electrodes

Julio J. Lado (Electrochemical Processes Unit, Madrid Institute for Advanced Studies, IMDEA Energy), Vincenzo Cartolano (Sanitary and Environmental Engineering Division (SEED), Department of Civil Engineering, University of Salerno), Enrique García-Quismondo (Electrochemical Processes Unit, Madrid Institute for Advanced Studies, IMDEA Energy), Yang Wang (School of Chemical Engineering and Technology, Tianjin University), Vincenzo Naddeo (Sanitary and Environmental Engineering Division (SEED), Department of Civil Engineering, University of Salerno), Jesús Palma (Electrochemical Processes Unit, Madrid Institute for Advanced Studies, IMDEA Energy), Marc A. Anderson (Electrochemical Processes Unit, Madrid Institute for Advanced Studies, IMDEA Energy)

### Abstract

Capacitive Deionization (CDI) is an emerging technology for brackish water desalination. Currently, CDI technology lacks practical means of scaling electrodes from the laboratory to pilot plant level for pre-commercial applications. With the aim of solving the scalability issues, we have prepared easy to scale 3D composites using the highly conductive macrostructure of a graphite felt (GF) as electron transfer channel with the microstructure of activated carbon (AC) to furnish ionic adsorption sites (GF-AC). The electrochemical characterization of GF-AC showed a larger total ion storage capacity as compared to an AC film electrode prepared with the same active material. GF-AC was then tested in a 1-Cell CDI System (10 cm<sup>2</sup>) reaching salt adsorption capacity ( $\rho_{SAC}$ ) values of 5.2-8.7 mg g<sup>-1</sup>, 57- 67% in charge efficiency and stable long-term operation (30% loss after 120 cycles). Finally, the system was scaled to a 9-Cell Stack (300 cm<sup>2</sup>) and tested using different operational modes (batch and single pass), parameters (flow, current density and voltage limit) and electrolyte concentrations (7 mM, 20 mM and 37 mM). Results in terms of productivity (2–47 L h<sup>-1</sup> m<sup>2</sup>) and energy consumption (0.1-0.7 kWh m<sup>-3</sup>) associated to salt concentration reductions (0.5- 10.0 mM) evidence the versatility of CDI technology.



### Biography: Julio J. Lado

Dr. Julio J. Lado Garrido holds a Ph.D. degree in Chemistry by Alcalá University (2014). Dr. Lado performed his PhD in IMDEA-Water research institute in collaboration with the University of Wisconsin-Madison (UW-Madison). In 2014 he obtained a postdoctoral fellowship from CAPES to join Luis A.M. Ruotolo group at the Federal University of São Carlos (Brazil). In 2017 he got a Talento postdoctoral fellowship from Comunidad de Madrid to work at IMDEA Energy. The core of his work is focused on the Water-Energy Nexus paying special attention to electrochemical ion separation processes such as capacitive deionization and battery desalination.

## 375 | Microbial reduction of organosulfur compounds in bioelectrochemical systems

Margo Elzinga (Wageningen University and Research), Dandan Liu (Wageningen University and Research), Jan Klok (Wageningen University and Research), Pawel Roman (Wetsus, European Centre of Excellence for Sustainable Water Technology), Cees Buisman (Wetsus / Wageningen University & Research), Annemiek ter Heijne (Wageningen University and Research)

### Abstract

Organosulfur compounds, present in e.g. the pulp and paper industry, biogas and natural gas, need to be removed as they potentially affect human health and harm the environment. The treatment of organosulfur compounds is a challenge, as an economically feasible technology is lacking. In this study, we demonstrate that organosulfur compounds can be degraded to sulfide in bioelectrochemical systems (BES). Methanethiol, ethanethiol, propanethiol and dimethyl disulfide were supplied separately to the biocathodes of BES, which were controlled at a constant current density of 2 A/m<sup>2</sup> and 4 A/m<sup>2</sup>. The decrease of methanethiol in the gas phase was correlated to the increase of dissolved sulfide in the liquid phase. A sulfur recovery as sulfide of 64% was found over 5 days with an addition of 0.1 mM methanethiol. Sulfur recoveries over 22 days with a total organosulfur compound addition of 1.85 mM was 18% for methanethiol and ethanethiol, 17% for propanethiol and 22% for dimethyl disulfide. No sulfide was formed in electrochemical nor biological control experiments, demonstrating that both current and microorganisms are required for the conversion of organosulfur compounds. This new application of BES for degradation of organosulfur components may unlock alternative strategies for the abatement of anthropogenic organosulfur emissions.

### Biography: Margo Elzinga

Margo Elzinga is a third year PhD student at Wageningen University and Research. She obtained her bachelor's degree in environmental sciences at van Hall University of Applied Sciences and her master's degree in water technology at the Wetsus Academy. She studies the (bio-)degradation of organosulfur compounds in bio electrochemical systems and is generally interested in biological conversions at biocathodes.

## 194 | Some specific operating features of PEMFC with binary fuel at low temperatures

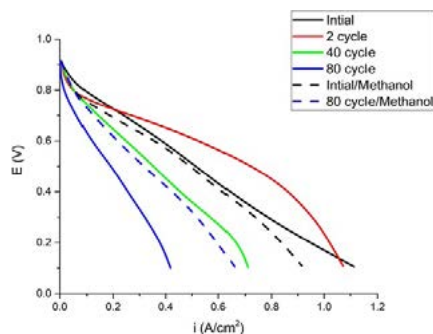
Nataliya Ivanova (National Research Center "Kurchatov Institute", 1, Akademika Kurchatova sq., Moscow 123182, Russia), Vladimir Fateev (National Research Center "Kurchatov Institute", 1, Akademika Kurchatova sq., Moscow 123182, Russia), Dmitry Spasov (National Research Center "Kurchatov Institute", 1, Akademika Kurchatova sq., Moscow 123182, Russia), Sergey Ostrovskiy (National Research Center "Kurchatov Institute", 1, Akademika Kurchatova sq., Moscow 123182, Russia), Ekaterina Seregina (National Research Center "Kurchatov Institute", 1, Akademika Kurchatova sq., Moscow 123182, Russia), Ruslan MenSharapov (National Research Center "Kurchatov Institute", 1, Akademika Kurchatova sq., Moscow 123182, Russia), Adelina ZasyPKina (National Research Center "Kurchatov Institute", 1, Akademika Kurchatova sq., Moscow 123182, Russia)

### Abstract

The main problem of PEMFCs operation at low temperature is MEAs degradation caused the water freeze-thaw process in a membrane and catalytic layers. This effect reduces PEMFCs performance. The first freeze-thaw led to a shortlived increase in the I-V characteristic by 10-15% (see fig.) due to some increase of the membrane volume. Subsequent freeze-thaw (range from +20 to -35 °C) cycling showed a significant decrease in MEAs performance: 35% loss after the 40th cycle and 55% loss after the 80th cycle. According to SEM-result after 80 cycles the catalytic layer had the structure with large pores and grooves, partially destroyed and separated from the membrane. The membrane structure was also destroyed, and the resistivity increased. In the case of the application of methanol additions to the hydrogen fuel, we observed an increase of a membrane liquid capacity without real changes in volume resistivity. The polymer material became more elastic and the liquid phase freezing temperature decreased. A complex-study showed that the catalytic layer degradation slows down almost twice and loss in MEAs performance was only 30% (by 80th freeze-thaw cycle) with methanol.

### Acknowledgements

The study was supported by NRC "Kurchatov Institute" (directive 1919, 25.09.2020, subprogram 6) and RFBR (№ 18-29-23030).



## 124 | Tunable Ion Selectivity in Capacitive Deionization with Prussian Blue Analogues

Kaustub Singh (Wetsus / Wageningen University & Research), Rafael Zornitta (Wageningen University and Research), Louis de Smet (Wetsus / Wageningen University & Research)

### Abstract

Selective removal of ions from water via capacitive deionization (CDI) is of relevance in applications such as water softening and purification, heavy metal removal and resource recovery. Intercalation materials like Prussian Blue Analogues (PBAs) have been used as an electrode material in an electrochemical CDI cell for selective ion separation. These materials have well-defined lattices with interstitial sites where cations intercalate according to their hydrated size. Here we present a vanadium based PBA as an ion-selective electrode for CDI. Explored only as a battery material, this PBA exhibits a selectivity of dual nature when used in treatment of ionic mixture in CDI. Unlike the size-based preference reported for PBAs, these electrodes prefer the larger divalent ions over smaller monovalent ions from a mixture of Li<sup>+</sup>, Na<sup>+</sup>, Ca<sup>2+</sup> and Mg<sup>2+</sup>. This trend is contrary to those in literature for PBAs in which smaller monovalent ions were preferred over the bigger divalent ions. However, VHCF does exhibit a size-based selectivity from an ionic mixture containing only monovalent or divalent ions. A two-step selectivity of this nature has never been previously reported for PBAs. This interesting property can help tailor CDI systems according to the application resulting in highly customizable route to ion selectivity.

### Biography: Kaustub Singh

Kaustub Singh is a PhD candidate in the theme of Capacitive Deionization at Wetsus. He is affiliated with and located at the department of Organic chemistry at Wageningen University, The Netherlands.

## 108 | Interaction of $\text{H}_3\text{PO}_3$ with Pt in concentrated $\text{H}_3\text{PO}_4$ electrolyte at elevated temperatures

Martin Prokop (University of Chemistry and Technology, Prague), Tomas Bystron (University of Chemistry and Technology, Prague), Martin Paidar (University of Chemistry and Technology, Prague), Karel Bouzek (University of Chemistry and Technology, Prague)

### Abstract

Proton-conductive membranes based on polymer/ $\text{H}_3\text{PO}_4$  composite are frequently utilised as an electrolyte in a medium temperature fuel cell technology. These fuel cells generally utilise Pt catalyst on electrodes and operate with  $\text{H}_2$  as a fuel and  $\text{O}_2$  as an oxidant within temperature range of 120 to 180 °C.

The limited electrochemical and chemical stability of  $\text{H}_3\text{PO}_4$  on a Pt surface at elevated temperatures is a long known issue.  $\text{H}_3\text{PO}_4$  is reduced, either chemically by the  $\text{H}_2$ , or electrochemically, to phosphorus impurities subsequently adsorbed on a Pt surface. Although one of the major products of this reduction was proven as  $\text{H}_3\text{PO}_3$ , exact nature of impurities and their electrochemical behaviour remains largely undescribed. Even in the case of  $\text{H}_3\text{PO}_3$ , electrochemical studies at directly relevant conditions are scarce in the literature.

The goal of this work is to describe electrochemical behaviour of  $\text{H}_3\text{PO}_3$  on a bulk Pt electrode in concentrated  $\text{H}_3\text{PO}_4$  electrolyte at temperatures above 120 °C. This comprises study of  $\text{H}_3\text{PO}_3$  formation and oxidation, as well as determination of an extent of  $\text{H}_3\text{PO}_3$  adsorption on a Pt surface at corresponding temperature.

### Acknowledgement

This study was supported by the Grant Agency of the Czech Republic under project No. 19-02964J.

### Biography: Martin Prokop

Dr. Martin Prokop finished his doctoral studies in 2018 in University of Chemistry and Technology, Prague under supervision of Prof. Karel Bouzek. During his doctoral studies, he worked for 5 months in Forth Institute of Chemical Engineering Sciences, Patras, under supervision of Dr. Stylianos Neophytides. From 2018, he works in postdoc position in Department of Inorganic Technology at University of Chemistry and Technology, Prague. His primary area of interest lies in general electrochemistry with specialisation in fuel cell field.

## Plenary: Learning the Physics of Batteries from Image Data

*Martin Z. Bazant*

*Departments of Chemical Engineering and Mathematics, Massachusetts Institute of Technology*

### Abstract

Traditional methods of scientific inquiry and engineering design begin with human intelligence: Mathematical models encoding physical hypotheses are proposed, tested against experimental data and refined by fitting adjustable parameters. Recent advances in artificial intelligence appear to challenge this paradigm, since predictions can be made directly from data without the need for models, but such knowledge is often not transferrable to new situations. This talk will present a hybrid approach of solving PDE-constrained inverse problems to derive useful chemical engineering models, in the particular context of Li-ion batteries. Examples of learning physics from image data include inferring electro-autocatalytic reaction models from x-ray diffraction spectra for NMC oxides, optical videos of lithium metal growth on graphite, and x-ray adsorption imaging of driven phase separation in LFP, as well as inversion of impedance spectra to determine microstructural heterogeneity, and acoustic emission spectra to reveal degradation processes during battery forming.

## 101 | Electrocatalytic Reaction Driven Flow

Abimbola Ashaju (University of Twente), Jeffery Wood (University of Twente), Rob Lammertink (University of Twente)

### Abstract

Bimetallic nanorods in form of microswimmers within an aqueous solution exhibits self-propulsion that is powered by self-electrophoresis. This bimetallic catalytic system can be immobilized to generate convective flow thereby acting as a micropump. In this work, we focus on experimental and numerical analysis that provides fundamental insight on the key elements including the generated electric field, reaction kinetics and diffusio-electroosmotic phenomena that control the resulting mass transport characteristics in these systems. The catalytic current between the electrodes and the induced potential that governs the reactive fluxes are measured electrochemically, proton concentration gradients originating from the catalytic reaction are imaged and quantified using fluorescence lifetime imaging, while the fluid flow is visualized with 3D particle tracking. Numerical simulations reveals the interplay of electrodes surface reactivity pattern represented by the dimensionless Damköhler number, with the electrokinetic phenomena that controls the release and depletion of protons and consequently the resulting induced fluid flow. This work highlights the ability of surface induced convective fluid flow in electrochemical systems to reduce mass transport limitations.

### Biography: Abimbola Ashaju

Abimbola Ashaju is a PhD student currently working on a transport phenomena project that can be harnessed in systems to reduce mass transport limitations. More details can be found at <https://research.utwente.nl/en/persons/abimbo-la-ayodeji-ashaju>

## 615 | Electrochemical Reduction of Nitrate over Bimetallic Catalysts in Aqueous Solutions: Effect of crystal structure and surface morphology

Jenn Fang Su (Department of Chemical and Materials Engineering, Tamkang University), Chin-Pao Huang (Department of Civil and Environmental Engineering, University of Delaware, Newark, DE)

### Abstract

Nitrate is a micronutrient and a potential carcinogen. Its removal from drinking water is essential to safe guard the public and ecological health. Previous studies have demonstrated that nitrate reduction in acidic solution is fast and easy toward the formation of ammonium final product. However, nitrate reduction to environmentally benign molecular nitrogen is necessary in order to control water quality in totality. This presentation will discuss our strategy on electrode preparation as to manipulate nitrate reactivity and nitrogen selectivity in electrochemical nitrate reduction. The preparation of tin-palladium electrodes was attempted using electrode deposition approach on stainless steel support. Different electrodeposition programs, such as charging processes and composition of metal solution affected the crystal structure and surface morphology of bimetallic electrodes, thereby impacted nitrate reduction capability. Based on XRD and analysis of reaction products, nitrate reduction over the synthesized Sn-Pd bimetallic electrodes was surface-structure sensitive; the fraction of (420) crystal facet of the Sn<sub>3</sub>Pd alloy exhibited critical effect on the reactivity and selectivity of nitrate reduction. Of the most significance, electrode prepared with one batch of solution containing both SnCl<sub>2</sub> and PdCl<sub>2</sub> at molar ratio of 1 to 4 exhibited the best performance in nearly 100% nitrate conversion and 81% nitrogen yield.

### Biography: Jenn Fang Su

J. F. Su is an Assistant Professor in the Department of Chemical and Materials Engineering at Tamkang University, Taiwan. She received her Ph.D. in Civil and Environmental Engineering from the University of Delaware, in Newark, Delaware, USA (2017). Prof. Su's research foci are on environmental materials and electrochemical technology aiming at selective conversion of hazardous wastes to value-added chemicals through nanocatalysts in aqueous phase. The overall goal is to understand the mechanism of electrochemical transformation of inorganic chemical species such as nitrate and provide a rational design for engineering nanocatalyst in wastewater treatment application.

### 15 | Enhanced fouling mitigation of conductive membrane electrode by electro-repulsion and in-situ electrocleaning in an electro-membrane reactor (EMR)

Jingqiu Sun (State Key Laboratory of Environmental Aquatic Chemistry, Research Center for Eco- Environmental Sciences, Chinese Academy of Sciences)

#### Abstract

A conductive graphene hydrogel membrane (GHM) was prepared by the compaction of graphene hydrogel under external pressure, whose pore size was stable at ~100 nm under various reduction degree. The stability of GHM under various redox states was beneficial for the electro-control of the membrane fouling without destruction of pore structure. The GHM was directly connected to the power source and worked as a membrane for separation and an electrode to control the membrane fouling. The cleaning time, electrolyte concentration and pollutant concentration were investigated for the electro-cleaning flux recovery rate of GHM, as well as the corresponding irreversible pollution ratio. Lower contaminants, higher electrolyte concentration and electrocleaning time were beneficial to recover the flux. The irreversible pollution ratio could be decreased to  $1.0 \pm 1.4\%$ . When the GHM was negatively charged, the membrane fouling was alleviated by the electro-repulsion and in-situ electro-oxidation. By controlling the electrode reaction, it was clarified that the mechanism of fouling mitigation was electro-repulsion and in-situ electrooxidation. And the electro-repulsion played a major role (83.01%) in comparison with the insitu electro-oxidation (16.99%). These findings laid a basic foundation for the development and application of the EMR system using electroconductive membrane.

#### Biography: Jingqiu Sun

Research Assistant of Research Center for Eco- Environmental Sciences, Chinese Academy of Sciences. His research interest focuses on the water treatment with no chemical additive and low maintenance by electrochemical method and membrane separation process.

### 338 | Development of a scrubbing processes using absorbents-electrolytes to the elimination of volatile organic contaminants

Florymar Durán (University of Castilla-La Mancha)

#### Abstract

The volatility of a lot of compound pesticides and industrial organic solvents favors their transfer to atmosphere, affecting importantly to the sustainability of ecosystems. For this reason, in recent decades, interest in the development of strategies capable to mitigate this problem has increased [1]. Scrubbing technology is known to be an efficient separation technology to remove gaseous pollutants and, recently, it has been proposed its combination with oxidation technologies that allow the regeneration of the absorbent-electrolyte. Formulation of this absorbent is a key input to reach high efficiencies and in the literature, it is reported the use of solutions containing precursors of Ag(II), Co(III) and Ce(IV) for the degradation of several air pollutants [2]. The combination of these processes is called electro-scrubbing technology. However, although this technology has made important contributions for the degradation of a lot of air pollutants, there are few studies on the organic volatile compounds in liquid phase as starting material.

This work focuses on the degradation of organic pollutants using absorbents-electrolytes containing metallic redox pairs, electrochemically generated in different diamond coatings as anodes. Results demonstrate that this technology can face their removal efficiently and regenerated the absorbent avoids the use of an excess of reagent.

#### Biography: Florymar Durán

Degree in Chemistry from the University of Los Andes Mérida- Venezuela.

Currently Ph.D. student in Chemistry from the Federal University of Rio Grande do Norte (Brazil) in cotutelle agreement with the University of Castilla - La Mancha (Spain) under the tutelage and responsibility of the following professors:

For the University of Castilla-La Mancha: Dr. Manuel Andrés Rodrigo Rodrigo, of the Department of Chemical Engineering in the doctoral program of Chemical and Environmental Engineering,

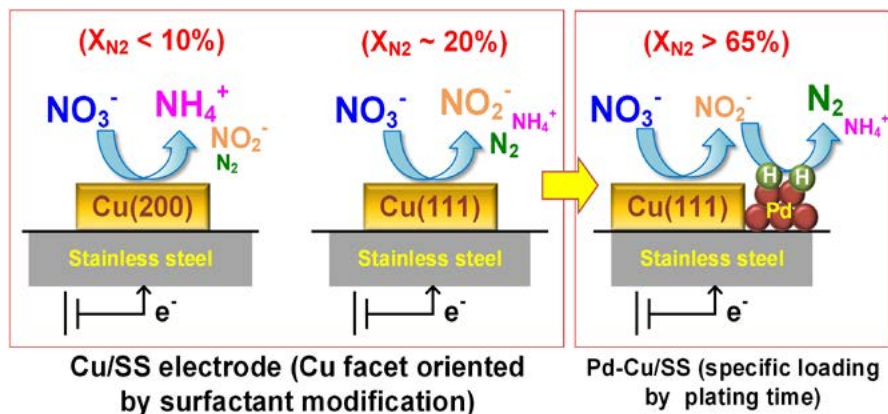
For the part of Federal University of Rio Grande do Norte: Dr. Carlos Alberto Martínez Huilte, of the Department of Chemistry.

### 331 | Electrochemical reduction of nitrate over Cu and Pd- Cu nanocatalysts as affected by crystalline morphology and facet

YuJen Shih (National Sun Yat-sen University), Chin-Pao Huang (Department of Civil and Environmental Engineering, University of Delaware, Newark, DE)

#### Abstract

Inorganic nitrogen, typically nitrate ( $\text{NO}_3^-$ ), nitrite ( $\text{NO}_2^-$ ) and ammonia ( $\text{NH}_3$ ), derived from degradation of organic-N, are essential micronutrients. The nitrogen concentration as low as 1-2 mg-N L<sup>-1</sup> can trigger eutrophication. This work tested two hypotheses: (1) metallic catalysts consist of one hydrogen active metal and one oxygen affinitive metal was more efficient than monometallic catalysts in nitrate reduction, and (2) crystal facet played a role on nitrate reactivity and selectivity. Surfactants, cetyltrimethylammonium chloride (CTAC), polydiallyldimethylammonium chloride (PDDA), and benzethonium chloride (BZT) were used to modify the crystal growth of metallic Cu nanoparticles supported on stainless steel (SS). X-ray diffractometer (XRD), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS) revealed the crystallographic shape and surface property of Cu nanoparticles. The first electron step was initiated at the onset potential of -0.6 V vs. Hg/HgO due to reversible Cu(0)/Cu(I) redox reaction, at which the electron transfer occurred favorably on Cu(200). The Cu(200)/Cu(111) ratio determined selectivity of  $\text{NO}_2^-$  and  $\text{NH}_4^+$ . The rate of  $\text{N}_2$  conversion was related to Cu(111), and substantially enhanced via the surface hydrogenation of Pd on bimetallic Pd-Cu/SS. High  $\text{N}_2$  yield ( $X_{\text{N}_2} = 0.65$ ) was observed over Pd<sub>0.27</sub>Cu<sub>0.73</sub>/SS synthesized using BZT at one critical micelle concentration (1xCMC).



#### Biography: YuJen Shih

To study the water and wastewater treatment in terms of electrochemical process, particularly aiming at the material science effects on redox reaction of decontaminating the pollution in solution.

### Plenary: Material recovery from end-of-life batteries

Xiaochu Wie, Sze-yin Tan, Anna Hankin and Geoff Kelsall  
Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK  
g.kelsall@imperial.ac.uk

#### Abstract

Lead-acid battery (LAB) production accounts for >85% of ca. 10 Mt a<sup>-1</sup> global lead usage, with LABs deployed in ca.  $1.3 \times 10^9$  vehicles. Accounting for > 85 % of total secondary Pb produced, LAB recycling is dominated by energy-intensive pyrometallurgical processes emitting CO<sub>2</sub> from carbonaceous fuels used for PbO reduction; additionally, lead's toxicity requires expensive gaseous and liquid pollution abatement. Hence, efficient and sustainable electro-hydrometallurgical LAB recycling technologies have been developed, some aspects of which will be described.

Exponential growth of lithium-ion battery production is causing concern about supplies of lithium compounds, providing motivation to develop material recovery processes for end-of-life lithium batteries. Ceramic lithium-ion conductors, such as  $\text{Li}_3\text{xLa}_{2/3-x}(1/3-2\text{x})\text{TiO}_3$  (LLTO), developed for prospective solid state lithium batteries, could also enable separation of lithium ions from other positive electrode components after dissolution in aqueous solutions. However, as membrane ionic conductivities are ca.  $5 \times 10^{-2} \text{ S m}^{-1}$ , ohmic potential losses may cause specific electrical energy consumptions to be uneconomic, unless thicknesses are constrained to  $\leq 10^{-4} \text{ m}$ , so such membranes require porous substrates to provide mechanical support. Results will be presented of electrolyte synthesis and fabrication, together with impedance measurements in aqueous solutions, indicating instability due to spontaneous lithium-ion dissolution.

### 564 | Monitoring Catalytic Changes by Microkinetic Modelling of the Oxygen Evolution Reaction

Janis Geppert (Karlsruhe Institute of Technology, Institute for Applied Materials – Electrochemical Technologies), Philipp Röse (Karlsruhe Institute of Technology, Institute for Applied Materials – Electrochemical Technologies), Ulrike Krewer (Karlsruhe Institute of Technology, Institute for Applied Materials – Electrochemical Technologies)

#### Abstract

Electrocatalytic water splitting is a highly promising reaction in order to produce “green” hydrogen. A benchmark material to catalyse the oxygen evolution reaction (OER) is rutile structured IrO<sub>2</sub> due to its high stability and reasonable activity in an acidic environment[1]. A better understanding of the changes of its complex surface chemistry is crucial for practical applications, especially during the operation up to several hours. Therefore, microkinetic modelling is a powerful tool to study reactions and limiting processes during dynamic operation[2,3]. In our work, we present an experimentally validated microkinetic model that allows to study the catalytic system. By balancing the reaction rates, active Ir surfaces sites are calculated to be covered mostly by adsorbed \*O (54 %) and \*OOH (26 %) species at typical OER potentials. Further, model-based parameter identification is conducted at several timesteps during the operation at OER conditions. Our monitoring analysis shows that the decay in OER current is not correlated to neither a change in pH, electrolyte resistance nor a lower amount of active surface sites. Lowered activity is rather affected by a change in selective thermodynamic energy barriers of deprotonation steps. Our method, thus, allows to bridge the gap between ab initio calculations and experiments.

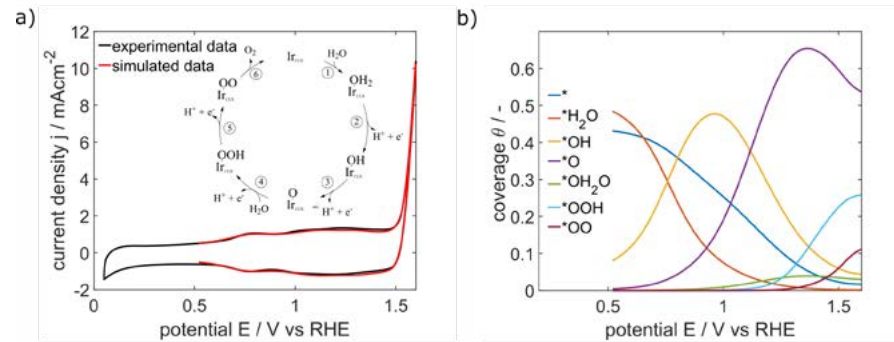


Figure 1: a) Experimental and simulated cyclic voltammogram based on the electrochemical mechanism (inset) of IrO<sub>2</sub> in 0.1 M H<sub>2</sub>SO<sub>4</sub>. b) Corresponding predicted coverage of adsorbed intermediate states during cycling.

#### Biography: Janis Geppert

2018 - today: PhD student at Technische Universität Braunschweig and Karlsruhe Institute of Technology, Germany  
 2018: M.Sc. in Physics at University Göttingen, German  
 2014: B.Eng. in Physics engineering at Trier University of Applied Sciences, Germany

### 614 | Transport and adsorption of organic micropollutants in reverse electro dialysis

Lingshan Ma (Ghent university), Leonardo Gutierrez (Ghent university), Marjolein Vanoppen (Ghent university), Arne Verliefde (Ghent university), Emile Cornelissen (Ghent university)

#### Abstract

Reverse electro dialysis (RED)-based hybrid processes (e.g., RED-ED/RO) have been proposed for more energy-efficient desalination in drinking water production. The use of secondary-treated wastewater as a low-salinity stream in RED raises concerns about enhanced membrane fouling and, especially, potential organic micropollutants (OMPs) contamination. The influence of membrane fouling and channel clogging on the transport and adsorption of 25 OMPs in RED was investigated using synthetic and real seawater and secondary-treated wastewater for 40 days. Real wastewater induced more membrane fouling and channel clogging than its synthetic counterparts and real seawater, as evidenced by pressure drop increase, permselectivity decrease, and ATP levels increase on membranes and spacers. The OMP transport and adsorption in real seawater conditions were higher than their synthetic counterparts, while OMP transport and adsorption under real wastewater conditions decreased significantly compared to synthetic wastewater conditions, possibly due to: 1) higher OMP-membrane interaction compared to OMPfouling layer interaction (steric and electrostatic mechanisms), and 2) OMP adsorption onto the effluent organic matter in real wastewater. These results provide critical implications for industrial scenarios. Specifically, OMPs transport might be overestimated at the lab-scale when using synthetic streams, clearly indicating the key role of effluent organic matter and fouling in RED using wastewater.

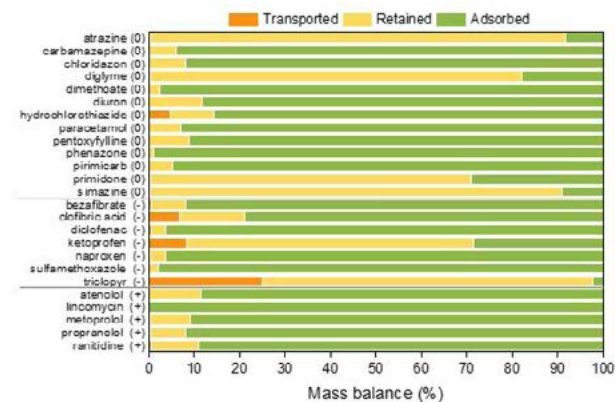


Figure. OMP transported (%) to seawater, retained in wastewater, and adsorbed in the system (transported + retained + adsorbed = 100%).

#### Biography: Lingshan Ma

Lingshan Ma is a PhD student working at Particle and Interfacial Technology Group of Ghent University. Her work is focusing on selective separation of inorganics and organics using ionexchange membrane technologies.

## 573 | Redox Exsolution: A Novel Bottom-Up Catalyst Preparation Method for Efficient Electrochemical Energy Applications

Vasileios Kyriakou (University of Groningen), Dragos Neagu (Strathclyde University), Michail Tsampas (Dutch Institute For Fundamental Energy Research)

### Abstract

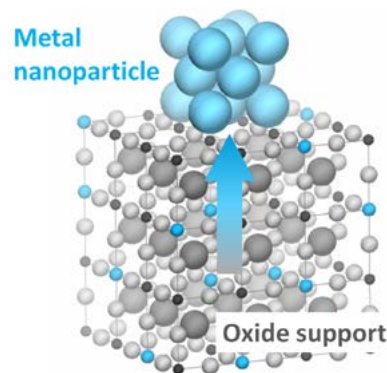
Functional materials consisting of metallic particles dispersed on the surface of oxides have been instrumental in enabling various catalytic and energy conversion applications. In the last decade, a novel preparation route called exsolution has emerged whereby the catalyst is substituted into the crystal lattice in ionic form and released upon reduction of the host oxide. Understanding and controlling the formation of nanoparticles is critical for tuning activity and stability. Here, we discuss fundamental aspects<sup>1</sup> and a new application<sup>2</sup> of the method.

By using a latest generation environmental TEM to follow the exsolution of individual nanoparticles, with ultra-high spatial and temporal resolution. Our analysis reveals the atomic scale processes that underpin the formation of the socketed, strain-inducing interface that confers exsolved particles their exceptional stability and reactivity. We then exemplify how exsolution can be employed to increase the efficiency of the renewable electricity-powered CO<sub>2</sub>/H<sub>2</sub>O solid oxide co-electrolysis, which is considered a promising technology for producing syngas feedstock. We also report on the use of exsolution to achieve the synergistic combination of coelectrolysis with CH<sub>4</sub> partial oxidation in a single cell.

### References

[1] D. Neagu et al, ACS Nano,13 (2019) 12996.

[2] V. Kyriakou et al, ACS Catalysis,10 (2020) 1278.



### Biography: Vasileios Kyriakou

Dr. Vasileios Kyriakou is an Assistant Professor at the University of Groningen. He holds a PhD in Electrochemical Process Engineering and a Diploma in Chemical Engineering from Aristotle University of Thessaloniki. He was a postdoctoral at the Department of Nuclear Science & Engineering of MIT and the Dutch Institute for Fundamental Energy Research. Dr. Kyriakou has published 36 peer-reviewed articles on fields such as electrochemical reaction engineering and heterogeneous catalysis. His current research focuses on the development of electrochemical devices and processes that convert and store renewable electricity into industrially attractive chemical fuels, such as ammonia and synthesis gas.

## 461 | Identification of rate determining step for OER and ORR in solid oxide electrochemical cell

Michal Carda (University of Chemistry and Technology, Prague), Daniel Budáč (University of Chemistry and Technology, Prague), Karel Bouzek (University of Chemistry and Technology, Prague), Martin Paidar (University of Chemistry and Technology, Prague)

### Abstract

High temperature reversible solid oxide cells (RSOCs) are a very promising technology for accomplishing the Hydrogen economy concept. High operating temperature brings RSOCs multiple benefits including favourable physicochemical conditions for hydrogen production and ability to operate in both electrolytic and fuel cell mode. Fast degradation is one of the biggest drawbacks of RSOCs. The cell design and working conditions of RSOCs have to be optimized to mitigate the degradation processes in order to make RSOCs more competitive in practical use. In order to be able to perform the optimization it is required to understand electrode reaction mechanism. Description of reaction scheme is quite challenging because there are at least three reaction steps including sorption/desorption, surface transport and charge transfer and more than one reaction pathway are possible. There may be also an impact of electrolyte microstructure on reaction pathway and rate determining step. It is well-known that an activity of oxygen vacancies is higher on grain boundaries than in their bulk. Still there is contradiction over an impact of grain boundary fraction on RSOC performance. Experiments with monocrystalline YSZ electrolytes were conducted to clarify the contradiction.

### Acknowledgements

Financial support of the Czech Science Foundation (contract No: 19-14244J) is acknowledged.

### Biography: Michal Carda

Michal Carda, the presenting author, is a Ph.D. student at Department of Inorganic Technology, at University of Chemistry and Technology in Prague. He graduated from the University of Chemistry and Technology in Prague in the study program: "Hydrogen and Membrane Technologies" (diploma thesis: "The influence of selected phosphorus compounds on H<sub>3</sub>PO<sub>4</sub>-doped proton exchange membrane fuel cell operation"). His Ph.D. research is focused on the high temperature electrochemical reactors for energy storage such as high temperature solid oxide cells.

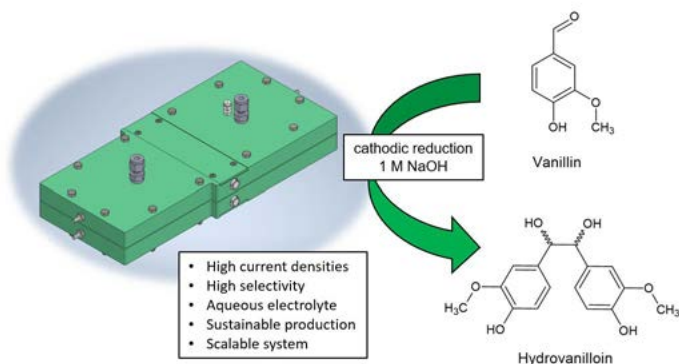


## 562 | Electrochemical Vanillin Reduction in a Flow Reactor: A Route to Biobased Polymers

Robin Kunkel (Fraunhofer Institute for Chemical Technology ICT), Volkmar M. Schmidt (Mannheim University of Applied Sciences), Fabian Simmat (HiTec Zang GmbH), Detlef Schmiedl (Fraunhofer Institute for Chemical Technology ICT), Jens Tübke (Fraunhofer Institute for Chemical Technology ICT)

### Abstract

Recently the field of biobased polymers has drawn much attention due to environmental concerns regarding existing petrochemical processes. Electrochemical cathodic conversion of vanillin and vanillin derivatives, one of the only biobased aromatic compounds available on an industrial level, enable a green process chain for the production of new biobased polymers and polymer building blocks. The main cathodic reaction product of vanillin in aqueous alkaline solution is the pinacolization product hydrovanillin, which is due to its bisphenolic structure of high interest in polymer synthesis. State of the art are batch cells at small scales for synthetic applications. For an industrial relevant scale, a transfer to an electrochemical flow reactor is required, which we addressed in this work. First, the mass transport of the system was characterized and enhanced by inserting in-house 3D-printed turbulence promoters. Further, the cathodic reduction of vanillin was investigated in detail and a simple model was developed to predict conversion rates up to constant current densities of 50 mA cm<sup>-2</sup>. The vanillin concentration was monitored by an online UV-Vis setup. This study provides a first step to a scalable system for the electrochemical production of vanillin-based polymer building blocks contributing to the transition to a sustainable future.



### Biography: Robin Kunkel

Robin Kunkel obtained his B.Sc. in chemical technology in 2016 and his M.Sc. in chemical engineering in 2018 from the Mannheim University of Applied Sciences. He did his masterthesis in the field of fuel cells at the Fraunhofer Institute of Chemical Technology ICT in Pfinztal. There he is currently a PhD student under the supervision of Prof. Tübke and Prof. Schmidt, working on the electrochemical synthesis of biobased polymers from vanillin. His PhD studies are supported by a Kekulé Fellowship of the Funds of the Chemical Industry.

## 540 | Comparison of electrochemical and vacuum ultraviolet (VUV)-based oxidation processes for cooling tower blowdown treatment -a case study

Pradip Saha (Wageningen University and Research), Harry Bruning (Wageningen University and Research), Huub Rijnaarts (Wageningen University and Research)

### Abstract

Cooling tower blowdown (CTBD) contributes to a large fraction of industrial water consumption. In this study, electrochemical (EO-AOP) and vacuum ultraviolet (VUV-AOP) advanced oxidation processes were assessed for dissolved organic carbons removal from CTBD to prevent membrane fouling during subsequent desalination. Particular attention was paid to the COD/TOC removal efficiency and the formation of organic and inorganic chlorinated by-products at three different pH values (pH=3, 7, 10). The results show that EO-AOP reached around 60% TOC removal and complete COD removal after 5 hours of treatment at 190mA applied current. A large amount of ClO<sub>x</sub>- and AOX were formed during EOAOP treatment, associating with the treated water's high micro-toxicity. A weak influence of pH on EO-AOP was demonstrated. Contrarily, pH strongly affected VUV-AOP, presenting outstanding TOC and COD removal under acidic condition (pH=3) while poor performance at pH10. The ClO<sub>x</sub>-- or AOX formation was limited in VUV-AOP process regardless of the value of the pH. Furthermore, the structural change of humic substances in CTBD water before and after each AOP treatment was also explored to understand the processes. Together, the information collected revealed that both AOPs can successfully be applied for removing dissolved organic carbon from CTBD water streams.

### Biography: Pradip Saha

Pradip Saha completed bachelor and master degree in Chemical Engineering & Polymer Science from Bangladesh. He worked in industries and university for seven years. Then, Pradip did his second master's degree in Environmental Technology (ETE) at Wageningen University and Research (WUR). In 2016, he started his PhD research in ETE at WUR, Netherlands in NOW-STW Water Nexus programme. His PhD is about technology integration for the removal of organic pollutants and salts from industrial wastewater.

## 192 | Oxygen reduction reaction at conducting polymer electrodes: Insights from DFT modeling

*Viktor Gueskine (Laboratory of Organic Electronics, ITN, Linköping University), Mikhail Vagin (Laboratory of Organic Electronics, ITN, Linköping University), Xavier Crispin (Laboratory of Organic Electronics, ITN, Linköping University), Igor Zozoulenko (Laboratory of Organic Electronics, ITN, Linköping University)*

### Abstract

Oxygen reduction reaction on gold in alkaline solutions - The inner or outer sphere mechanisms in the light of recent achievements.

Conducting polymers as electrodes are attracting increasing attention due to their possible role in transition to greener and more sustainable production methods. The experimental feasibility of such key electrochemical processes as hydrogen evolution and oxygen reduction reactions (HER and ORR) at *p*-type polymer PEDOT and *n*-type polymer BBL, in the absence of any metal impurities, has been demonstrated in this laboratory and by others. Mechanisms of electrochemical reactions *at* conducting polymer electrodes is a subject more complex than electrochemistry *of* conducting polymers themselves. In particular, the mechanisms of electrocatalytic reactions can hardly be transposed from those established e.g. for platinum, so the very role of a conducting polymer electrode remains uncertain.

In this communication, we expose our methodology and key recent findings from our DFT based modelling of ORR at PEDOT and BBL in aqueous electrochemical conditions. We demonstrate the role of a conducting polymer as a molecular material driving outer-sphere electron transfer, more similar to enzyme cofactors or gold electrodes rather than to oxygen chemisorbing electrodes. We discuss the practical implications of our modeling results.

### Biography: Viktor Gueskine

Dr Viktor Gueskine is group leader of Organic Electrodeics at Laboratory of Organic Electronics, University of Linköping, Sweden since 2018. He obtained PhD in physical chemistry at Russian Academy of Sciences and previously worked in research institutes and universities in Russia, France, and Belgium. He is a specialist in electrochemistry, atomic force microscopy, and computational chemistry, He is the author of 90 publications in international peer-reviewed journals, with over 2500 citations and H-index 27 (ORCID 0000-0002-7926-1283). His current scientific interests are centered at electrochemistry of conducting polymers, including applications and elucidation of reaction mechanisms.

## 103 | Simulation Modelling for Sustainable Large-scale Electroforming

*Eleni Andreou (University of Strathclyde), Sudipta Roy (University of Strathclyde)*

### Abstract

Electroforming is an electrochemical additive manufacturing process used to fabricate mechanically robust stress-free complex structures. Regardless its extensive empirical use, the scientific understanding of the process's parameters is limited. Our team aspires to contribute towards the realisation of this electrochemical additive manufacturing process in Industry 4.0 era.

Our approach uses scientifically informed design of the process that can lead to scale-up for volume manufacturing. To achieve this, the electrochemical properties of the system need to be mapped and their effect on the chemistry of the process needs to be explained. Data gathered through systematic physico-chemical and electrochemical analysis will provide the knowledge base to simulate the process and verify by experiments at a prototype electroforming setup, in-house.

To model the nickel deposition on a rotating steel disk that we will present, data on the pH, electrolyte conductivity, limiting current, reversible and irreversible potentials and mass transfer coefficients are of essence. Using this data as input parameters in COMSOL® software, a finite element method approach would allow the derivation of useful information leading to the optimisation of the currently used process parameters and/or the proposal of a new process model benefited by lower waste, lower inventoryrelated needs and optimised supply chain.

### Biography: Eleni Andreou

Eleni is currently a PhD candidate at the University of Strathclyde. She obtained her MEng in Chemical Engineering from the National Technical University of Athens, followed by a MSc in Chemistry from the University of Glasgow. Aspiring to enhance her background on electrochemical engineering and materials science, she joined the "Electrochemical and Corrosion Research Group" of Professor Sudipta Roy for her PhD studies.

Her current research focuses on the design, optimisation and simulation modelling of the industrial electroforming process of nickel and nickel alloys. The project is co-funded by the National Manufacturing Institute Scotland (NMIS) and Radius Aerospace - Bramah.

## 468 | Electrochemical process development for production of bio-based maleic acid

Roman Latsuzbaia (TNO), Saskia Bubberman (TNO), Amanda Garcia (TNO), Carlos Sánchez Martínez (TNO), Erwin Gilling (TNO), Mark Roelands (TNO), Earl Goetheer (TNO; TUDelft)

### Abstract

Maleic acid is an important chemical, which is used in variety of processes, such as in production of lubricants, plasticizers, pharmaceuticals and in production of bio-based aromatics. However, industrially produced maleic acid is fossil based. It is produced by hydrolysis of maleic anhydride, which on the other hand is produced by gas phase thermocatalytic oxidation of butane by oxygen catalyzed by vanadium-based V-P-O catalysts, with the process yields only 50-65% maleic anhydride. Alternatively, renewable maleic acid can be produced by electrochemical oxidation of bio-based furfural. Electrochemical oxidation allows selective and less energy demanding conversion at ambient pressures and temperatures using cheap catalysts, such as Pb/PbO<sub>2</sub>. Our research focused on scale-up of maleic acid production looking at reaction development utilizing a plate-and-frame type flow electrolyser, as well as product separation. The electrolysis was investigated directly on Pb/PbO<sub>2</sub> electrode, and the effect of mediators, electrolysis temperature and furfural concentration on conversion were investigated. Paired electrolysis options were investigated to improve process economics. Based on the obtained results techno-economic feasibility study has been performed and showed high potential for an economically favorable production.

### Biography: Roman Latsuzbaia

Roman Latsuzbaia obtained his PHD from Delft University of Technology on development of catalysts for PEM fuel cells in 2015. Since then he is working at TNO as a research scientist. Main responsibilities include research into development of electrochemical production processes of fine and bulk chemicals, examples involve electrochemical conversion of carbon dioxide and bio-based chemicals.

## 41 | Multistage reverse electro dialysis effect for energy generation

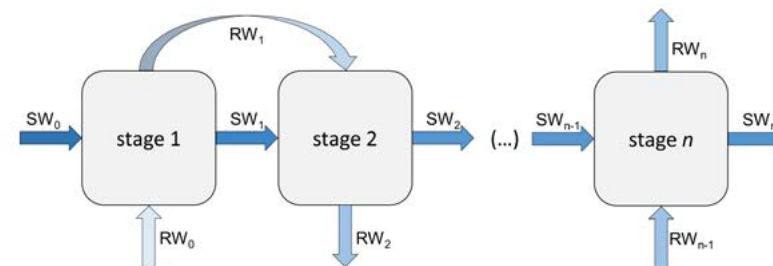
Catarina Simões (University of Twente), Pedro Ribeiro (Universidade Nova de Lisboa), Diego Pintossi (Eindhoven University of Technology), Michel Saakes (Wetsus), Svetlozar Velizarov (Universidade Nova de Lisboa), Wim Brilman (University of Twente)

### Abstract

Reverse electro dialysis (RED) can be used to harvest salinity gradient energy. For RED to become an economically attractive process, the feedwaters should be used to the maximum extent, particularly when pre-treatment costs are high. Furthermore, pumping costs should be minimized. Short residence times result in a high gross power density leading to a relatively low energy efficiency and higher pumping costs. Long residence times result in higher net energy efficiencies and low hydrodynamic losses, as ionexchange is further promoted. However, the power density output is strongly reduced due to less available energy per unit of time. Multistage RED (Figure 1), accomplished by feeding multiple stacks in series, can offer sufficient net energy efficiency while having a power density such that the process becomes economically viable.

To study the effect of multistage RED in cross-flow stacks, artificial seawater (30 g NaCl/L) and river water (1 g NaCl/L) were used. Residence time, number of stages, stages configuration and stacks size were studied experimentally.

The results when using two stages instead of a single stage, show a net energy efficiency increasing from 11.4 to 19.4 % while the net power density only decreases from 1.2 to 1.0 W/m<sup>2</sup>.



### Biography: Catarina Simões

Catarina Cerqueira da Silva Simões is PhD Candidate since October 2018 at Wetsus and in cooperation with the University of Twente. She obtained a master degree in Chemical and Biochemical Engineering from the NOVA University of Lisbon. Her master thesis was entitled "Bipolar membrane based energy storage system: the acid-base flow battery". Currently, she works on the scale-up of novel redox free concepts to optimize the reverse electro dialysis process for energy generation. She was granted a NPT award for the best Poster at the 16th Netherlands Process Technology Symposium.

### 63 | Mass transport effects on the electrooxidation of glycerol on electrodeposited palladium-nickel catalysts

Jai White (Department of Chemical Engineering, KTH Royal Institute of Technology, Teknikringen 42, SE-10044, Stockholm), Daniel Martin-Yerga (Department of Chemical Engineering, KTH Royal Institute of Technology, Teknikringen 42, SE-10044, Stockholm. Current affiliation: Department of Chemistry, University of Warwick, Coventry CV47AL, United Kingdom), Gunnar Henriksson (Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 56, SE-10044, Stockholm), Ann Cornell (Department of Chemical Engineering, KTH Royal Institute of Technology, Teknikringen 42, SE-10044, Stockholm)

#### Abstract

Clean fuel demands are increasing motivation for hydrogen to be a central component of the energy transition towards sustainable societies. Currently, water electrolysis dominates electricity driven hydrogen production. However, the anodic oxygen evolution reaction is kinetically limiting and only overcome with high energy input. The glycerol electrooxidation reaction (GEOR) provides a more thermodynamically favourable anodic reaction to produce hydrogen electrolytically. However, it is poorly understood in terms of mass transport, concentration and temperature effects on the activity of catalysts. Electrochemical valorisation of glycerol, a cheap by-product of biodiesel refineries, can contribute to closing the biomass resource cycle as hydrogen is used in the synthesis of ammonia-based fertilisers. Additionally, glycerol, a tri-hydroxyl functionalised alcohol, is a suitable platform chemical to contribute towards zero-pollution manufacturing as the GEOR products have valuable and important use in the medical, cosmetic and waste water treatment industries. This study, via rotating disk electrodes, evaluates the electrochemical performance effects of various temperatures and electrolyte concentrations (NaOH and glycerol) on electrodeposited palladium-nickel (PdNi) bimetallic catalysts on Ni disks. Highest glycerol oxidation currents were found at an intermediate electrode rotation rate, at high temperature and high NaOH concentration with the onset voltage almost half that required for oxygen evolution.

#### Biography: Jai White

Jai White received his B.Sc. and B.Math. degrees in Chemistry and Pure Mathematics from the University of Newcastle, Australia. From which he also obtained his Honours (First Class) degree in Chemistry researching the electrocatalysis of the nitrogen reduction reaction. He is a Ph.D. candidate in Applied Electrochemistry in the Department of Chemical Engineering at KTH, Royal Institute of Technology, Stockholm in Sweden. His current research interests include the electrocatalysis of the glycerol oxidation reaction on PdNi catalysts and how changes in mass transport, electrolyte concentration and temperature effect peak oxidation currents of such catalysts.

### 359 | Changing the configuration of an air-diffusion cathode reactor to operate Fenton-based treatments of organic pollutants in continuous mode

Anlin Xu (Nanjing University of Science and Technology), Weiqing Han (Nanjing University of Science and Technology), Enric Brillas (Universitat de Barcelona), Ignacio Sirés Sadornil (Universitat de Barcelona)

#### Abstract

Industrial additives like benzotriazole (BTR) pose environmental concerns due to their massive use and occurrence in water. Wastewater treatment technologies in conventional plants are ineffective to remove them. Within this context, electro-Fenton (EF) and photoelectro-Fenton (PEF) processes are envisaged as suitable alternatives to ensure their transformation into innocuous products. The key steps in EF and PEF are the insitu  $H_2O_2$  electrogeneration upon 2-electron  $O_2$  reduction and the continuous Fe(II) regeneration. The air-diffusion cathodes combine high efficiency and selectivity for  $H_2O_2$  electro-synthesis with relatively low cost due to the absence or minimization of metal-based catalyst loading. Here, a novel tubular electrochemical reactor, equipped with an air-diffusion cathode and porous Ti/RuO<sub>2</sub> anode, has been devised for the EF treatment of BTR in different matrices in continuous mode. Coupling with a photoreactor (PEF mode) enhanced the degradation. Continuous and stable  $H_2O_2$  production was confirmed at 10-40 mA cm<sup>-2</sup>. After the stabilization period, the best steady-state removals attained were 100% for BTR and 70% for total organic carbon (TOC), thus corroborating the interest of this reactor configuration.

#### Acknowledgements

Funding from CTQ2016-78616-R (AEI/FEDER, EU) and PID 2019-109291RB-I00 (AEI, Spain), as well as the PhD scholarship to A. Xu (State Scholarship Fund, CSC, China), is acknowledged.

#### Biography: Ignacio Sirés Sadornil

Ignacio Sirés Sadornil (Barcelona, Spain, 1980) obtained Bachelors in Chemistry (University of Barcelona, UB) and Materials Engineering (Polytechnic University of Catalunya, UPC). Prof. Enric Brillas supervised his PhD in environmental electrochemistry at the UB (PhD degree in Chemistry in January 2007). He carried out several postdoctoral stays, and then became Associate Professor at the UB in 2009. He has published more than 150 indexed articles (> 10000 citations,  $h_i = 48$ ), six book chapters and two patents, and has supervised six Doctoral Theses. In 2014 he was awarded the Carl Wagner Medal of Excellence in Electrochemical Engineering (WPEE-EFCE).

## 215 | Plasma activated electrolyser for nitrogen fixation by water

Rakesh Sharma (Dutch Institute For Fundamental Energy Research), Hrishikesh Patel (Dutch Institute For Fundamental Energy Research), Stefan Welzel (Dutch Institute For Fundamental Energy Research), Richard van de Sanden (Dutch Institute For Fundamental Energy Research), Michail Tsampas (Dutch Institute For Fundamental Energy Research)

### Abstract

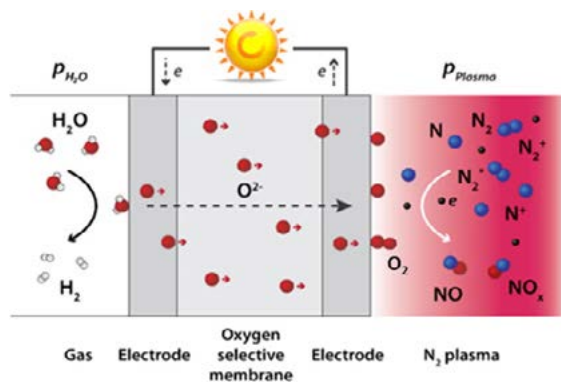
One of the greatest challenges of our era is the substitution of fossil-based energy sources with renewable ones. However, because of their intermittent nature and the harvesting in the form of electricity, their direct introduction into the value chain remains challenging. Therefore, technologies based on renewable electricity that can transform base molecules (i.e.,  $H_2O$ ,  $N_2$ ,  $CO_2$ ) have attracted tremendous interest.<sup>1,2</sup>

The main research question that has to be addressed urgently is the most effective way of converting electrical energy into molecules of high energy or chemical value. In the transition from low- to high-energy molecules or to valuable chemical feedstock, the activation of chemical bonds (e.g.,  $N=N$ ,  $O=C=O$ ) has to be tackled.

In this contribution, we will present a unique (allelectric) solution for overcoming material limitations, towards nitrogen fixation. We employ solid oxide electrolysis cells (SOECs) that allow us to provide reacting species on catalysts with a controllable manner while a radiofrequency plasma is used to increase the reactivity of nitrogen. By employing  $O_2^-$  or  $H^+$  conductor we can produce either  $NH_3$  or  $NO$  by suppressing  $H_2$  or  $O_2$  evolution reactions respectively.

### References

- [1] T.M. Gur, Energy Environ. Sci., 11 (2018) 2696  
 [2] H. Patel et al, ACS Energy Lett., 5 (2019) 2091



### Biography: Richard van de Sanden

M.C.M. (Richard) van de Sanden is professor in the Plasma and Materials Processing group of Eindhoven University of Technology and since 2011 director of Dutch institute For Fundamental Energy Research (DIFFER). At DIFFER he focuses on plasma-surface interaction under extreme nuclear fusion conditions, and conversion of solar energy into fuels and chemicals. He has (co)-authored over 450 papers in peer-reviewed journals, his h-index is 70, he has more than 20000 citations and is the co-inventor of >20 patents. He is a fellow of AVS, IUPAC and IOP and serves on numerous scientific committees of international conferences.

## 333 | Influence of Micrometric Inter-Electrodes Distance and Water Hardness on Mineral Scaling at Electrode Surface during Electrochemical Advanced Oxidation Process

Faidzul Hakim Adnan (Laboratoire Réactions et Génie des Procédés, Université de Lorraine, CNRS, LRGP, F-54000 Nancy, France), Emmanuel Mousset (Laboratoire Réactions et Génie des Procédés, Université de Lorraine, CNRS, LRGP, F-54000 Nancy, France), Marie-Noëlle Pons (Laboratoire Réactions et Génie des Procédés, Université de Lorraine, CNRS, LRGP, F-54000 Nancy, France)

### Abstract

In electrolytic water treatment, scaling or deposit is an inevitable challenge and it normally ends up in capital loss due to technical issues. When the electrode is polarized at a sufficiently negative potential, dissolved oxygen and water are reduced to hydroxyl ions. These two phenomena result in an increase of local pH at the vicinity of electrode. In presence of  $Mg^{2+}$  and  $Ca^{2+}$ , hydroxide scales can potentially be produced. On another side, this pH increment also shifts the thermodynamic ratio of carbonates/bicarbonates favoring the production of carbonate scales. The influence of reactor design on mineral scaling was investigated in this study by considering a microfluidic thinlayer cell in micrometric range compared to electrolyzer with inter-electrodes distance in centimeter range. Short distances have shown to enhance mass transfer within the cell and it overcomes the barrier of working with low ionic conductivity electrolyte.  $Mg(OH)_2$  and  $CaCO_3$  deposits were selected in this work, as they are the main scales encountered in the field. Coupling the experimental results with voltammetry and impedance spectroscopy allowed depicting the mechanism of nucleation and scaling. The applied current density range was larger with thin films to avoid scaling effect, which could enlarge the applications of micro-reactors.

### Biography: Faidzul Hakim Adnan

Faidzul Hakim Adnan is a second-year PhD student at LRGP (UMR 7274 CNRS/Université de Lorraine) in Nancy, France, working on the application of combination of nanofiltration and electrochemical advanced oxidation processes to treat wastewater. The supervisors (i.e. coauthors) are worldwide experts in the field. Dr. Emmanuel Mousset has been involved for 10 years with advanced oxidation and electrochemical processes for environmental applications, he presented 10 keynotes and was awarded the "Green Electrochemistry" Prize from ISE/Elsevier (2018). Dr. Marie-Noëlle Pons has long-term experience in water treatment with about 200 papers in peer-reviewed journals and more than 400 presentations in conferences.

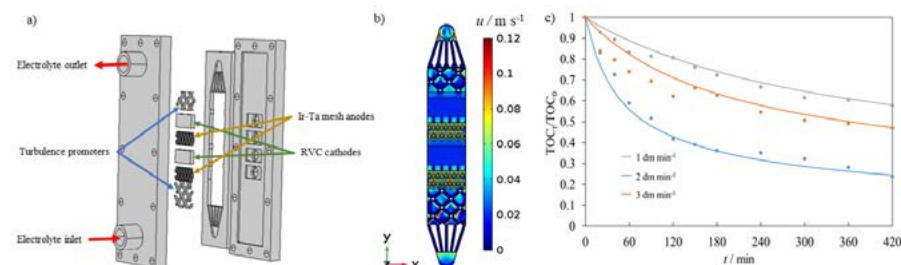
### 209 | Design and characterization of a novel flow-through electrochemical reactor for hydrogen peroxide electrosynthesis directed to the incineration of organic compounds by electrochemical advanced oxidation processes

Oscar Cornejo (Universidad de Guanajuato), José L. Nava (Universidad de Guanajuato)

#### Abstract

The presence of persistent organic pollutants POPs in different water bodies has increased with the growth of the industrial sector, which generates large quantities of wastewater. The most common POPs are dyes, pharmaceuticals, herbicides, fungicides, etc. In recent years, the electrochemical advanced oxidation processes (EAOPs) have become a proper way to incinerate these POPs from water up to carbon dioxide. These processes include the electro-Fenton, photo electro-Fenton and solar photo electro-Fenton, and the most recent electro-peroxone. These EAOPs produce hydrogen peroxide at the cathode, which react with  $\text{Fe}^{2+}$  or  $\text{O}_3$  to yield the hydroxyl radicals ( $\cdot\text{OH}$ ), which are the responsible to incinerate the POPs.

This work deals with the design and characterization of an electrochemical reactor to produce hydrogen peroxide at the cathode, with the oxygen generated at the anode, without the incorporation of any  $\text{O}_2$  external source. The  $\text{H}_2\text{O}_2$  is employed in the electroperoxone process to mineralize chloramphenicol, in a prepilot flow plant using the electrochemical cell coupled in series to a homogeneous reactor, where the peroxone reaction takes place. Computational fluid dynamics (CFD) simulations were performed to characterize the hydrodynamics, mass transport and current distribution (the reaction environment) of the process, Fig. 1.



**Figure 1.** a) Scheme of the Flow-through electrochemical reactor for hydrogen peroxide electrosynthesis; b) velocity field inside the channel of the electrochemical reactor obtained by the solution of the Navier-Stokes and Brinkman equation; and c) normalized total organic carbon (TOC) decay of a model molecule obtained by experimental (dots) and theoretical (solid lines) results.

#### Biography: Oscar Cornejo

Oscar M. Cornejo is a PhD student in University of Guanajuato under the guidance of Dr. José Luis Nava Montes de Oca. He obtained his chemical engineering bachelor's degree at University of Guadalajara while his MSc degree was obtained at the University of Guanajuato. His current research involves the design and characterization of electrochemical flow cells by computational fluid dynamics and wastewater treatment with electrochemical advanced oxidation processes.

### 199 | Advanced treatments for depleting non-polar organochlorine pesticides from concentrated sludges

Alexandra Raschitor (University of Castilla-La Mancha), Javier Llanos (University of Castilla-La Mancha), Gustavo Acosta-Santoyo (University of Castilla-), Erika Bustos (Centro de Investigación y Desarrollo Tecnológico en Electroquímica), Pablo Cañizares (University of Castilla), Manuel A. Rodrigo (University of Castilla-La Mancha)

#### Abstract

An alternative to increase the efficiency of electrochemical degradation processes is coupling them to a previous concentration stage. For the particular case of non-polar organochlorines, electrocoagulation can be used to produce a sludge with high concentration of the target pollutant.

This work presents two different possibilities of handling these sludges using integrated electrochemical techniques. The first approach was the pretreatment of the concentrated sludge by applying ultrasound irradiation (US) followed by electrooxidation. Secondly, electrochemical dewatering (ED) was used to obtain the maximum allowable dehydration of the sludge along with the oxidation of the pollutants.

By applying US, it was possible to brake the iron flocs, making the pollutant available for its depletion by electrolysis, obtaining removals degrees ranging from 15 to 95 %. Regarding electrochemical dewatering, it was possible to reduce the initial volume to less than 15 % withdrawing clean treated water. Moreover, with the proper electrode arrangement, it was possible to obtain simultaneously the degradation of the pollutant along with the dehydration of the sludge.

#### Acknowledgements

The financial support from the Spanish Ministry of Economy, Industry and Competitiveness through project CTM2016-76197-R (AEI/FEDER, UE) and the National Council for Science and Technology (CVU: 264785, Mexico) is gratefully acknowledged

#### Biography: Javier Llanos

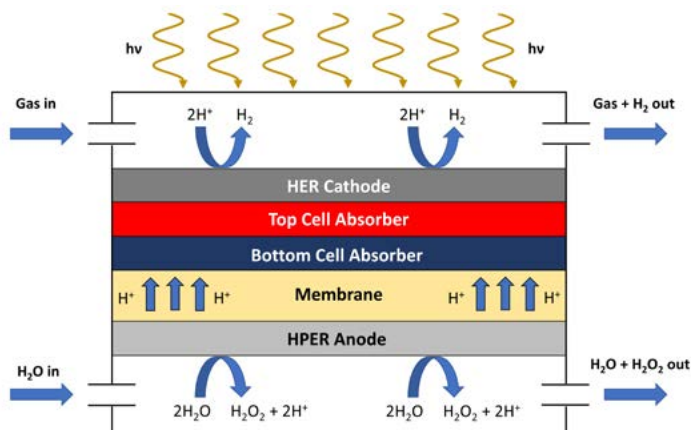
Chemical engineer from the University of Castilla- La Mancha (UCLM) in 2005, receiving the first national prize of Chemical Engineering. Doctoral Thesis at the same University, finished in March 2010. During the last 11 years, I have been part of the teaching staff of the Department of Chemical Engineering of the UCLM in different positions, currently as Associate Professor. Research experience developed in the Department of Chemical Engineering of the UCLM and through collaborations with five international excellence centres. Co-author of 80 JCR papers, with an H index of 24 and a citation record of 1513 cites according to Scopus.

## 189 | Towards anodic $\text{H}_2\text{O}_2$ production as a profitable commodity chemical in PEC water splitting

Kasper Wenderich (University of Twente), Wouter Kwak (University of Twente), Birgit Nieuweveme (University of Twente), Alexa Grimm (Utrecht University), Guido Mul (University of Twente), Bastian Mei (University of Twente)

### Abstract

To increase industrial interest in hydrogen production through photoelectrochemical (PEC) water splitting, substitution of oxygen with a valuable commodity chemical at the anode is a valid strategy. In this work, we first investigate the techno-economics of a PEC system with partial water oxidation to hydrogen peroxide ( $E^\circ(\text{H}_2\text{O}_2/\text{H}_2\text{O}) = +1.78 \text{ V vs RHE}$ ). We discuss (i) a scenario where an artificial leaf (see Figure) with optimal solar-to-hydrogen (STH) efficiency and Faradaic efficiency is used, and (ii) a literature-based state-of-the-art scenario consisting of a hybrid PEC/PV configuration using  $\text{BiVO}_4$  as a photoanode. For both scenarios, our analysis predicts lower hydrogen prices compared to 'classic' PEC water splitting. Competition with steam methane reforming can even be realistic under the right circumstances. In the second part of the presentation, experimental work on selective water oxidation to  $\text{H}_2\text{O}_2$  is discussed. We show that in a nonoptimized electrochemical cell, we can easily achieve continuously electrochemically production of  $\text{H}_2\text{O}_2$  at a rate of  $4.57 \mu\text{mol min}^{-1} \text{ cm}^{-2}$  @  $48.7 \text{ mA/cm}^2$ . We will discuss the importance of electrolyte, electrode and reactor engineering to enhance the Faradaic efficiency and the  $\text{H}_2\text{O}_2$  production rate.



### Biography: Kasper Wenderich

Kasper Wenderich (born in 1987 in Hengelo, The Netherlands) received his MSc in Applied Physics in 2011 at the University of Twente, the Netherlands. Afterwards, he continued as a PhD student at the Photocatalytic Synthesis (PCS) Group, also at the University of Twente, which he finished in 2016. In his PhD thesis, he studied the photocatalytic deposition of platinum nanoparticles on tungsten trioxide. After spending two years at the MLU Halle-Wittenberg in Germany, he returned to the PCS Group at the University of Twente for a second postdoc. He currently investigates the electrochemical production of hydrogen peroxide.

Award ceremony

## New views in the anodic oxidation of organics The Electrochemical Oxygen Transfer Reactions (EOTR)

Christos Comninellis

Swiss Federal Institute of Technology, Faculty of Basic Science  
EPFL-1015 Lausanne, Switzerland

Oxidative electrochemical processes promising versatility, environmental compatibility and cost effectiveness have a continuously growing importance both in selective organic synthesis and in the electrochemical incineration (ECI) of organic pollutants in aqueous media. In case of organic electrosynthesis selectivity is to be enhanced and in the ECI process the aim is the mineralization of the toxic and non-biocompatible pollutants with high current efficiency. Anodic oxidation of organics may proceed by several mechanisms including direct and indirect oxidation.

In direct electrochemical oxidation, electron exchange occurs between the organic species and the electrocatalytic electrode surface. A typical example is the oxidation of organic compounds (methanol) on platinum anodes at low anodic potentials. The main problem with electrocatalytic anodes of platinum group metals is the decrease of the catalytic activity during use when proceeding oxidation of organics at a fixed anodic potential, before oxygen evolution. This is mainly due to the adsorption of reaction intermediates (mainly CO) at the anode surface, commonly called poisoning effect.

In indirect electrochemical oxidation, the organics do not exchange with the surface directly but through intermediation of some electroactive species. This intermediation may be homogeneous or heterogeneous.

In this work the electrochemical oxidation of organics at DSA® type electrodes based on synthetic boron-doped diamond (BDD) and metal oxide anodes in acid medium are presented. Both the direct and indirect electron transfer reaction are discussed.

In case of facile outer-sphere electrode reactions, both BDD and oxide electrodes behave similarly to that of noble metal electrodes.

In oxidation reactions of more complex mechanism, these anodes show no activity below the potential of oxygen evolution and electrochemical oxygen transfer reactions (EO-transfer) can take place only in the potential region of water discharge.

A simplified mechanism of EOTR catalyzed by intermediates of oxygen evolution has been proposed distinguishing between two limiting electrode behaviors:

- At 'non-active' anodes (typically BDD and fully oxidized metal oxides)
- EO-transfer occurs at a high anode potential through physisorbed hydroxyl radicals.
- At 'active' electrodes ( $\text{IrO}_2$ ,  $\text{RuO}_2$ ) the reaction takes place at lower potentials
- and results in an EOTR through the higher oxidized metal oxide surface sites.

Finally a kinetic model of organics oxidation at 'non-active' and 'active' type anodes is proposed and confirmed by preparative electrolysis.

## List of posters

259	A. Anthes	<b>Purification of gadolinium- and platinum-containing pharmaceutical wastewater by an electrochemical controlled sorption process</b>
452	A. Arulrajan	<b>Exceptional Water Desalination Performance with Anion-Selective Electrodes</b>
280	I. Atlas	<b>Maximum available energy during desalination using chemical energy inputs</b>
608	G. Bampos	<b>Pd-Based Bimetallic Electrocatalysts for the Hydrogen Oxidation Reaction in Alkaline Medium</b>
296	Y. Belaustegui	<b>Three-dimensional reduced graphene oxide electrodes for capacitive deionization</b>
519	P. Berg	<b>Modelling transport phenomena in Nafion with a pore-network approach</b>
181	H. Bergmann	<b>Improvements in Calculating OH Radical Concentration Profiles at a BDD Anode for Water Electrolysis</b>
198	S. Bhandari	<b>Stabilizing Effect of Platinum on Iron-Based Electrocatalysts in Polymer Electrolyte Membrane Fuel Cells</b>
477	R. Bisselink	<b>Electrochemical conversion of acid hydrolysis products derived from sugars</b>
423	J. Blake	<b>Modelling of Gas Diffusion Electrode Catalyst Layers for CO<sub>2</sub> Reduction</b>
126	B. Branco	<b>Towards an up-scalable artificial leaf by integration of printing methodologies</b>
479	Y. Bultel	<b>Liquid/solid suspension in vanadium redox-flow battery</b>
214	T. Cadden	<b>Nanostructured Tungsten Oxide Architectures for Electrochemical Energy Storage</b>
534	K. Denk	<b>Membrane alkaline water electrolysis stack design and characterization</b>
272	S. Genthe	<b>Challenges of developing an electrically rechargeable zinc-air battery with a zero gap electrode arrangement</b>
499	S. Georg	<b>Role of fermentative hydrogen as electron donor in bio-electrochemical systems for nutrient recovery</b>
223	S. Gonzalez-Poggini	<b>Effect of Ti<sub>3</sub>C<sub>2</sub>Tx nanosheets (MXenes) in the electrocatalytic activity of SnO<sub>2</sub>/Ti anodes for the degradation of methyl red</b>
464	P. Bosch Jimenez	<b>Carbon nanofibers doped with metals for air-cathodes. Oxygen reduction reaction characterization and application in microbial desalination cells</b>
506	S. Kandhasamy	<b>Challenges behind long-term cyclability of Intermediate Temperature Sodium Sulfur (IT-NaS) Battery</b>
315	V. Karastoyanov	<b>Composition, electrical and optical properties of nanoporous TiO<sub>2</sub> doped with iron and molybdenum oxides</b>
308	R. Kupec	<b>ElektroDeHalo – Adsorption and electro-degradation of halogenated pollutants</b>
496	A. Laube	<b>Design and performance analysis of a tubular PEM electrolysis cell</b>
202	T. Lemmermann	<b>Development of standardized characterization routine for membranes in vanadium redox-flow batteries</b>
244	J. Llanos	<b>Strategies for increasing the efficiency of the electrochemical degradation of polar organochlorine pesticides</b>
492	A. Maćkowiak	<b>Deep Eutectic Solvents Based on Lithium Nitrate and Acetamide as Electrolytes in High-Temperature Electric Double-Layer Capacitors</b>
566	J. Mališ	<b>Investigation Of Changes In Potential Distribution In Pem Fuel Cell Stack At Different Content Of Impurities In Fuel</b>
113	A. Marquez	<b>Electrochemical Incineration of the Methyl Orange Textile Dye by Anodic Oxidation, Electro-Fenton and Photoelectro-Fenton Processes</b>
388	M. Martí Calatayud	<b>Concentration of organic acids by electrodialysis: identification of mass transfer phenomena by means of electrochemical impedance spectroscopy</b>
460	T. Matthée	<b>The ElectroSynthesis Starter Kit - Exploring Electrochemistry</b>
140	J. Mrlík	<b>Investigating the deactivation of negative felt electrode of vanadium redox flow battery</b>



279	F. Murrieta	<b>Electrochemical degradation of sulfamethoxazole by a Fenton-type process promoted by electrogenerated HClO and dissolved Fe<sup>2+</sup></b>
268	U. Mushtaq	<b>Development of proton conducting solid oxide electrolysis cell electrode tailored for CO<sub>2</sub> reduction into useful products.</b>
327	J. Nava	<b>Design and characterization of an interdigitated bipolar plate to be used in an AEM fuel cell</b>
262	M. Paidar	<b>Optimization of preparation of ceramic electrolytes based on ZrO<sub>2</sub>-Y<sub>2</sub>O<sub>3</sub> suitable for high temperature cells with ceramic oxides</b>
474	M. Mascia	<b>Experimental study on the optimisation of pollutants removal by photo-electrochemical oxidation with TiO<sub>2</sub> nanotubes</b>
567	R. Passalacqua	<b>NiFe Oxides as Anodic Materials for the Electrocatalytic Oxidation of Glucose to Glucaric Acid</b>
224	T. Montañés-Sanjuan	<b>Efficient removal of CVP by electrochemical oxidation using different anodes</b>
225	M. Martí Calatayud	<b>Influence of the presence of a cation-exchange membrane for electro-oxidation of CVP using BDD or low-cost ceramic anodes</b>
322	K. Plakas	<b>Electrochemical treatment of agrochemical manufacturing industry wastewater and landfill leachate</b>
539	M. Plevová	<b>Preparation of catalyst coated membrane for alkaline water electrolysis: influence of the substrate and preparation method</b>
549	P. Richtr	<b>Development of oxygen reduction and oxygen evolution electrodes for alkaline zinc-air flow battery</b>
597	A. Samu	<b>Effect of the operating parameters on electrocatalytic CO<sub>2</sub> reduction in a zero-gap cell</b>
275	B. Sánchez Batalla	<b>Tubulyze: tubular Proton Exchange Membrane water electrolysis cells</b>
377	C. Simões	<b>Electrode segmentation in reverse electrodialysis for energy generation</b>
552	S. Spiess	<b>Bioelectrochemical Methanation of CO<sub>2</sub> from Untreated Steel Mill Gas</b>
118	A. Sustronk	<b>How adding CO to CO<sub>2</sub> changes the performance of flow-through porous copper electrodes</b>
406	P. Thivel	<b>Study of lithium batteries ageing in aeronautics applications for second life purposes</b>
400	R. Uwayid	<b>Characterizing and mitigating the degradation of oxidized cathodes during capacitive deionization cycling</b>
553	E. van der Veer	<b>Ferroelectric lithography for energy harvesting</b>
554	A. Venger	<b>Structure of SIX2a, associated with electrocytes of Electrophorus electricus</b>
556	O. Venger	<b>Structure and ligands of EFA01355 protein of electric ray Torpedo nobiliana</b>
267	J. Záchenská	<b>Electrochemical preparation of nickel-based electrodes for HER in alkaline water electrolysis</b>
431	C.Ferchaud	<b>Solid Oxide Cell development at TNO for high temperature electrolysis</b>
003	E.Al-Dhubhani	<b>Performance of five commercial bipolar membranes under forward and reverse bias conditions for acid-base flow battery applications</b>
129	R. Sharifian	<b>Electrochemical oceanic CO<sub>2</sub> Capture</b>

# PalmSens 4™

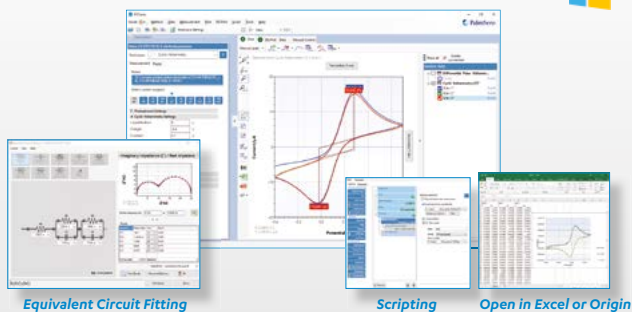
Potentiostat / Galvanostat / Impedance Analyzer



### Main Specifications:

- FRA / EIS: 10  $\mu$ Hz to **1 MHz**
- 9 current ranges: 100 pA to 10mA
- High resolution of 0.006% (full scale range)
- $\pm$  **10V** dc-potential range at 75  $\mu$ V resolution
- USB and battery powered
- Never lose data with **8 GB** internal storage

**PSTrace 5** (standard included): software for windows



[www.palmsens.com](http://www.palmsens.com)

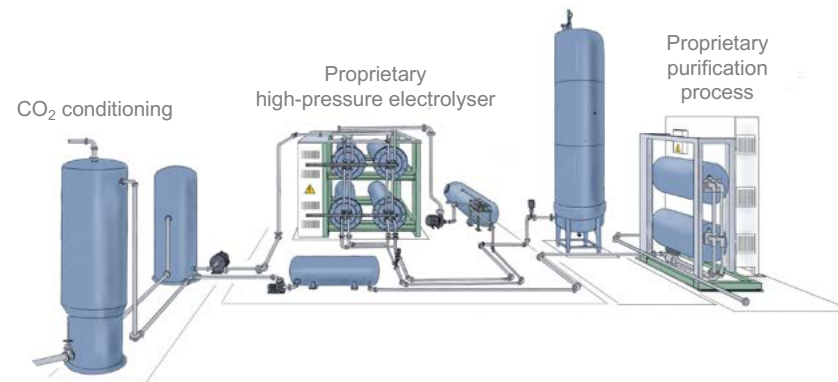


## COVAL Ventures

Developing ground-breaking CO<sub>2</sub> utilisation solutions



### Process Overview



#### Energy efficiency

Current efficiency	>80%
Cell voltage	3.2V
Current density	>50 mA/cm <sup>2</sup>

#### Status of technology

Fully funded to TRL7

#### Upscaling

Development of a pilot plant with 40 kg per day formate production

#### Opportunities

- Emerging applications including
- chloride-free de-icing liquid
  - sustainable fuels
  - energy storage
  - aquafeed

#### Challenges

Improving current density

#### Economics

Colyser production cost are within range of the market prices, underpinning the Colyser's economic viability

Contact

[Frank@covalenergy.com](mailto:Frank@covalenergy.com)

# IVIUM TECHNOLOGIES

innovative solutions for electrochemical research and testing towards electrification and energy transition for a greener society



POTENTIOSTATS/GALVANOSTATS

BATTERY TESTERS

INTEGRATED IMPEDANCE

MULTICHANNEL CONTROL SOFTWARE

DEDICATED DATA ANALYSIS SOFTWARE

DATASECURE/DATABASE STORAGE

IVIUM TECHNOLOGIES develops and manufactures a wide range of potentiostats and testers for a variety of applications. Our instruments range from entry level to high-end specifications, and include various multichannel potentiostats and battery test systems. We also offer portable potentiostats for mobile and field use. All our instruments include integrated FRA/EIS.

For our potentiostats we can offer a high-capacity data storage system to prevent data loss during longterm measurements. Potentiostat to PC connection can be established via USB, Ethernet and WIFI.

Our instruments are controlled via our powerful yet intuitive IviumSoft user control software. This is supplied free of charge with each instrument, for unlimited installs. IviumSoft includes both single and multichannel instrument control and data-analysis, as well as a sophisticated battery cycling and testing module.

Various performance enhancing modules, power boosters and peripheral functionality upgrades are available.

Contact Ivium:

Ivium Technologies  
De Zaale 11  
5612AJ Eindhoven  
The Netherlands

tel.: +31 (0)40 239 0600  
mail: [info@ivium.com](mailto:info@ivium.com)  
web: [www.ivium.com](http://www.ivium.com)

Hi-Tech Detection Systems

## CLEAN WATER ?

### Find it out with our electrochemical solutions

Potentiostats / Galvanostats

Battery testers and analyzers

Local electrochemistry

Portables solutions, electrodes and accessoires

**Reliable and cost-saving solutions for your most demanding electrochemical applications**

**Suivez nous !**

[www.htds.fr](http://www.htds.fr)  
[info@htds.fr](mailto:info@htds.fr)

Contact: Sr Pierre-Julien VOISIN, pierre-julien.voisin@htds.fr; +33 (0) 6 03 76 09 51

# VIONIC powered by INTELLO

One instrument, pure discovery for all your electrochemical research



Highest combined specifications in one single instrument

Compliance voltage:  $\pm 50$  V  
Standard current:  $\pm 6$  A  
EIS frequency: up to 10 MHz



[www.metrohm.co.uk](http://www.metrohm.co.uk)