NPS19

Netherlands Process technology Symposium

Bridging Sustainable Process and Product Technology

8 & 9 October 2024

Book of Abstracts

Forum Groningen | Nieuwe Markt 1 | 9712 KN Groningen

Table of Content

Word of Welcome

We hope you enjoy reading this program book for the 19th edition of the Netherlands Process technology Symposium (NPS 19) to be held in Forum Groningen on 8 to 9 October 2024.

NPS 19 is the leading event to highlight academic achievements in the Netherlands and beyond in chemical engineering and related fields. It provides a great opportunity to connect academia, industry, and society. The theme of NPS 19 is “Bridging sustainable process and product technology”. The development of sustainable processes and the design and manufacture of environmentally benign (bio-based) chemical products are key to addressing societal challenges. The program is a combination of plenary talks, keynote lectures, and oral and poster presentations

Jun Yue, Hero Jan Heeres,

Paolo P. Pescarmona, Jingxiu Xie, Vassilis Kyriakou

Timetable

8th of October

Time	Room			
	NOK	Camera 4	Camera 1	Rabo Studio
08:30 - 09:00	Registration (Forum Atrium, Ground Floor)			
09:00 - 10:45	Opening, Welcome and Plenary I & II (Rabo Studio)			
10:45 - 11:15	Coffee Break (Atrium)			
11:15 - 12:30	Parallel 1.1 Renewable carbon conversion	Parallel 1.2 (Bio)chemical Process Engineering	Parallel 1.3 Electrochemical Engineering *(incl. Keynote 1)*	Parallel 1.4 Design of (Bio)chemical Products & Materials *(incl. Keynote 2)*
12:30 - 13:30	Lunch Break (Atrium)			
13:30 - 14:45	Parallel 2.1 Process Systems Engineering	Parallel 2.2 (Bio)chemical Process Engineering *(incl. Keynote 3)*	Parallel 2.3 Reaction and Catalytic Engineering	Parallel 2.4 Separation Technology & Transport Phenomena *(incl. Keynote 4)*
14:45 - 15:15	Coffee Break (Atrium)			
15:15 - 16:00	Plenary III (Rabo Studio)			
16:00 - 17:00	Poster Parade & Sponsor Pitch (Rabo Studio)			
17:00 - 18:30	Poster Session & Welcome Reception (Atrium)			
19:00 - 22:00	Conference Dinner (Rabo Studio)			

9th of October

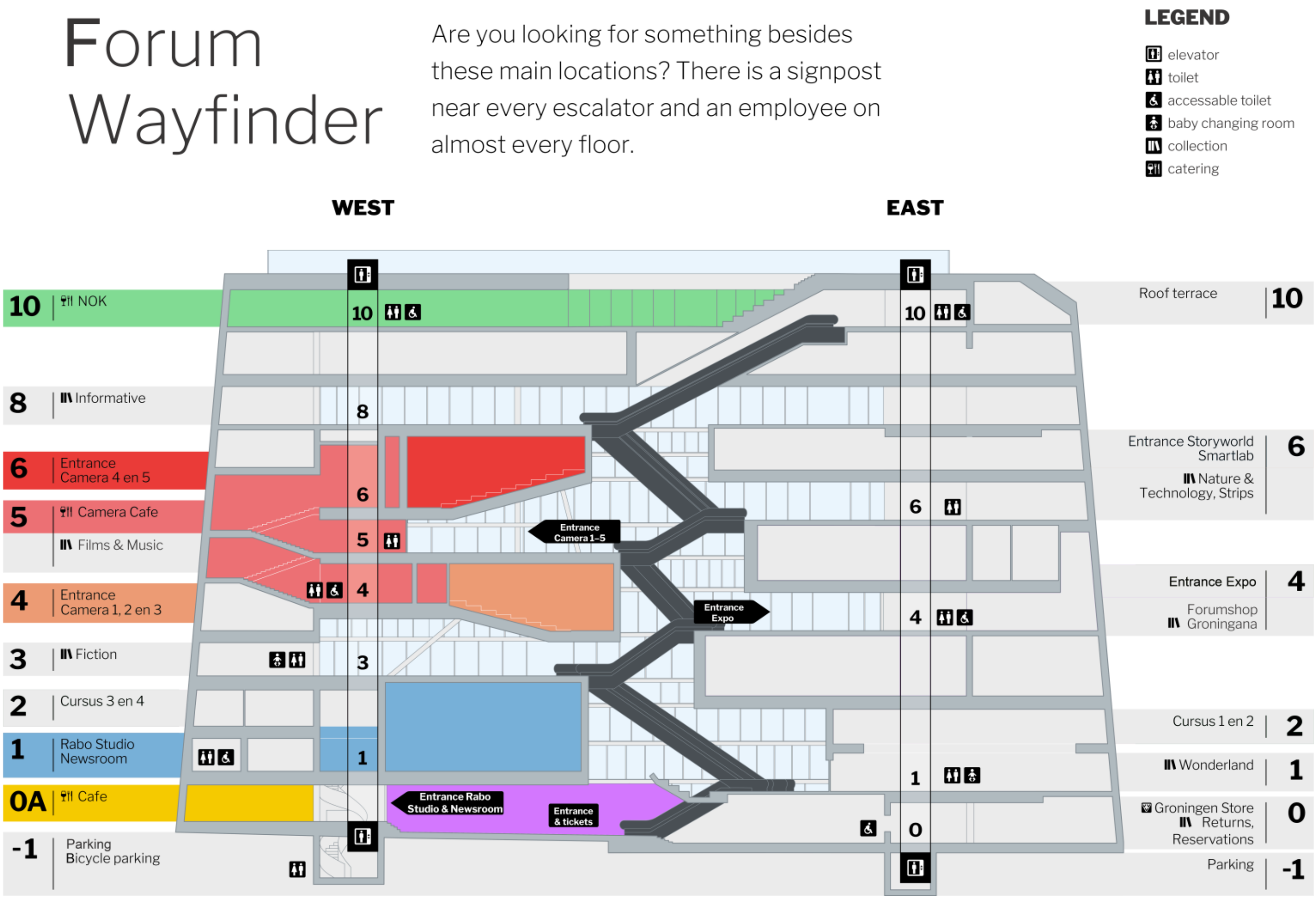
Time	Room			
	NOK	Camera 4	Camera 1	Rabo Studio
08:30 - 09:00	Registration (Forum Atrium, Ground Floor)			
09:00 - 10:00	Announcements and Plenary IV (Rabo Studio)			
10:00 - 10:45	Poster Parade (Rabo Studio)			
10:45 - 11:15	Coffee Break (Atrium)			
11:15 - 12:30	Parallel 3.1 Process Systems Engineering *(incl. Keynote 5)*	Parallel 3.2 (Bio)chemical Process Engineering	Parallel 3.3 Electrochemical Engineering	Parallel 3.4 Separation Technology & Transport Phenomena
12:30 - 13:45	Lunch Break and Poster Session (Atrium)			
13:45 - 15:00	Parallel 4.1 Renewable carbon conversion	Parallel 4.2 Reaction and Catalytic Engineering *(incl. Keynote 6)*	Parallel 4.3 Electrochemical Engineering	Parallel 4.4 Separation Technology & Transport Phenomena
15:00 - 15:30	Coffee Break (Atrium)			
15:30 - 16:30	Hoogewerff Gold Medal Ceremony and Lecture Plenary V (Rabo Studio)			
16:30 - 17:00	Awards & Closing Ceremony (Rabo Studio)			

Venue & Map

Venue

NPS 19 will be hosted in the Forum Groningen (Nieuwe Markt 1, 9712 KN Groningen), right in the city center of Groningen. It is within twenty minutes walking distance from the central station of Groningen, but there are also bus connections. Please check the 9292 website for more information on the bus connections and schedules.

Map of Forum Groningen



Theme and topics

The theme of NPS 19 is “Bridging sustainable process and product technology”, centered around 7 topics:

- Renewable carbon conversion
- (Bio)chemical Process Engineering
- Electrochemical Engineering
- Design of (Bio)chemical Products & Materials
- Reaction and Catalytic Engineering
- Separation technology & Transport Phenomena
- Process System Engineering

Instructions for presenters

Please contact the chair of your session 10 minutes prior to the start of your parallel session. Please also make sure that you upload and test your presentation.

Plenary
Timing: 40 minutes presentation + 5 minutes discussion

Keynote
Timing: 25 minutes presentation + 5 minutes discussion

Oral
Timing: 12 minutes presentation + 3 minutes discussion

Poster
A0 Poster

Poster & sponsor pitch
Maximum 3 slides (pitch presentation of 90 seconds)

Scientific & Organization Committee

7

We would to thank the scientific and organization committees for taking the time to read and rate all the abstracts submitted to NPS 19.

Scientific committee

- Atsushi Urakawa
- Chiara Gualandi
- Edwin Zondervan
- Fausto Gallucci
- Martin van Sint Annaland
- Sepas Setayesh
- Thijs de Groot
- Wiebren de Jong

Local organization committee

- Jun Yue
- Hero Jan Heeres
- Paolo P. Pescarmona
- Jingxiu Xie
- Vassilis Kyriakou

Program Oral Presentations 8

8th & 9th of October

Monday 7th of October 2024

NPS Business Dinner (by invitation only)

From 19:00 to 22:00, Prinsenhof

Tuesday 8th of October 2024

Registration

From 8:30 to 9:00, Forum (Ground floor)

Welcome and Plenary Lecture I & II

From 9:00 to 10:45, Forum (Rabo Studio)

Chaired by: Jun Yue & Jingxiu Xie

9:00 **Opening and welcome**

9:15 **[PL01] Title:** The long road of scaling renewable chemical process technology. The Avantium story on how to bring the new, plant-based polyester PEF to market
Presenter: Tom van Aken (Avantium)

10:00 **[PL02] Title:** From Applications to Fundamentals: The Power of Multiscale Modelling
Presenter: Raffaella Ocone (Heriot-Watt University)

Coffee Break

From 10:45 to 11:15, Forum (Ground floor)

Parallel Session 1.1 Renewable Carbon Conversion

From 11:15 to 12:30, Forum (NOK)

Chaired by: Peter Deuss

11:15 **[OP01] Title:** Biphasic furfural synthesis from biorefinery feed using coated 3D foam structures
Presenter: Adarsh Patil (Eindhoven University of Technology)

11:30 **[OP02] Title:** Transformation of glucose to 5-hydroxymethylfurfural over $AlCl_3$ catalyst in water: the effect of choline chloride addition
Presenter: Chencong Ruan (University of Groningen)

11:45 **[OP03] Title:** Power-to-Methanol: techno-economical evaluation of a digestion use-case
Presenter: Hans Gelten (Saxion University of Applied Science)

12:00 **[OP04] Title:** Synthetic kerosene from CO_2-rich synthesis gas via Fischer-Tropsch synthesis
Presenter: Bart C.A. de Jong (University of Groningen)

12:15 **[OP05] Title:** Highly Active and Selective Borophene based catalysts for Reverse Water Gas Shift Reaction
Presenter: Rajamohanan Sobhana Anju (University of Amsterdam)

Parallel Session 1.2 (Bio)chemical Process Engineering

From 11:15 to 12:30, Forum (Camera 4)

Chaired by: Peter de Jong

11:15 **[OP06] Title:** Supercritical CO_2 as effective wheat straw pretreatment for subsequent mild fractionation strategies
Presenter: Salvador Bertran-Llorensa (University of Groningen)

11:30 **[OP07] Title:** Oxidative pretreatment as a way of upgrading cellulose-rich municipal waste streams
Presenter: Ana Luiza Slama de Freitas (University of Groningen)

11:45 **[OP08] Title:** Complete liquefaction of enzymatic hydrolysis lignin via non-catalytic solvolysis
Presenter: Xiang Li (Aalto University)

12:00 **[OP09] Title:** A Sustainable Process Design For The Production of Nitrile Butadiene Rubber for Medical Glove Usage
Presenter: Shivam Pandey (Delft University of Technology)

12:15 **[OP10] Title:** Generative artificial intelligence (AI) in chemical process engineering
Presenter: Artur M. Schweidtmann (Delft University of Technology)

Parallel Session 1.3 Electrochemical Engineering

From 11:15 to 12:30, Forum (Camera 1)

Chaired by: Peter Veenstra

11:15 **[OP11] Title:** Understanding the Selectivity of Bicarbonate Electrolysis
Presenter: Iris Burgers (Delft University of Technology)

11:30 **[OP12] Title:** Modification of stainless-steel as bifunctional electrocatalysts towards high active and stable anion-exchange membrane water electrolysis
Presenter: Tao Jiang (University of Groningen)

11:45 **[OP13] Title:** A computational study on the impact of electrolyzer geometry on the Faradaic efficiency of alkaline water electrolyzers
Presenter: Bryan Acosta-Angulo (Eindhoven University of Technology)

12:00 **[KL01] Title:** Membrane electrolysis: essential for chemicals; enabler for sustainable process and product development
Presenter: Hans Lammers (Nobian Industrial Chemicals B.V.)

Parallel Session 1.4 Design of (Bio)chemical Products & Materials

From 11:15 to 12:30, Forum (Rabo Studio)

Chaired by: Ruud van Ommen

11:15 **[KL02] Title:** Design of sustainable polymeric products
Presenter: Francesco Picchioni (University of Groningen)

11:45 **[OP14] Title:** Improved colloid stability of polymer microspheres by low temperature deposited nanofilms of SiO_2 in fluidized beds
Presenter: Rens Kamphorst (Delft University of Technology)

12:00 **[OP15] Title:** Preparation and Selected Applications of Polymer Thin Films Synthesized by Initiated Chemical Vapor Deposition (iCVD)
Presenter: Yizeng Di (University of Groningen)

12:15 **[OP16] Title:** Diels Alder and domino reactions for self-healing materials
Presenter: Paul van den Tempel (University of Groningen)

Lunch Break

From 12:30 to 13:30, Forum (Ground floor)

Parallel Session 2.1 Process System Engineering

From 13:30 to 14:45, Forum (NOK)

Chaired by: Meik Franke

13:30 **[OP17] Title:** Techno-economic and environmental impacts of replacing fossil-based processes in the propylene subcluster in the Port of Rotterdam
Presenter: Inna Stepchuk (Delft University of Technology)

13:45 **[OP18] Title:** Exploring the synergistic integration of CO_2 electrolysis and CCS supply chains for sustainable syngas production
Presenter: Thijmen Wiltinka (Delft University of Technology)

14:00 **[OP19] Title:** Numerical and Experimental Study of the Axis-Switching Phenomena in Rectangular Jets
Presenter: Cristina García Llamas (Eindhoven University of Technology)

14:15 **[OP20] Title:** Systematic methodology via a decision matrix for the quick selection of energy-efficient intensified distillation technologies
Presenter: Qing Li (Delft University of Technology)

14:30 **[OP21] Title:** Modelling and Analysis of Electrolysers Integrated with Downstream Separation Systems via Heat Pumps
Presenter: Riccardo Dal Mas (Delft University of Technology)

Parallel Session 2.2 (Bio)chemical Process Engineering

From 13:30 to 14:45, Forum (Camera 4)

Chaired by: Gert-Jan Euverink

13:30 **[KL03] Title:** Without process innovation no protein transition
Presenter: Peter de Jong (ISPT)

14:00 **[OP22] Title:** Performance assessment for the Twente-DAC pilot using sorbent circulation.
Presenter: Abhinav Srinivas (University of Twente)

14:15 **[OP23] Title:** Coprecipitation of magnetite nanoparticles using a liquid/liquid Membrane Reactor
Presenter: Negar Amani Tehrani (Eindhoven University of Technology)

14:30 **[OP24] Title:** Techno-economic assessment of a decentralized system for pure hydrogen production via green ammonia decomposition
Presenter: Valentina Cechetto (Eindhoven University of Technology)

Parallel Session 2.3 Reaction and Catalytic Engineering

From 13:30 to 14:45, Forum (Camera 1)

Chaired by: Wiebren de Jong

13:30 **[OP25] Title:** The shape-dependent activity of Pd/CeO_2 nanorods, nanocubes, and nano-octahedrons on lean methane oxidation
Presenter: Martim C. Policano (University of Twente)

13:45 **[OP26] Title:** Integrated process development for the conversion of lignocellulosic biomass to ethylene glycol
Presenter: Romolo Di Sabatino (University of Twente)

14:00 **[OP27] Title:** Morphology controlled ceria catalysts for reverse water gas shift reaction (RWGS)
Presenter: Pankaj Verma (University of Amsterdam)

14:15 **[OP28] Title:** Enhancing Methane Oxidation in Maritime Engines: A Numerical Study of Pre-Reactor Temperature Control
Presenter: Julian C. Restrepo (University of Twente)

14:30 **[OP29] Title:** Novel internal fin configurations for gas-liquid monolithic reactors
Presenter: Aniket S. Ambekar (Eindhoven University of Technology, Technical University of Munich)

Parallel Session 2.4 Separation Technology & Transport Phenomena

From 13:30 to 14:45, Forum (Rabo Studio)

Chaired by: Raffaella Ocone

13:30 **[OP30] Title:** Calibration of pore network models via inverse gas chromatography
Presenter: David Rieder (Eindhoven University of Technology)

13:45 **[OP31] Title:** A coupled Local Front Reconstruction and Immersed Boundary Method for simulating multiphase flows with contact line dynamics
Presenter: Tom Janssen (Eindhoven University of Technology)

14:00 **[OP32] Title:** Pressure drop of single- and two-phase flows in single pellet string microreactors: the influence of wall effect
Presenter: Lu Zhang (University of Groningen)

14:15 **[KL04] Title:** Microfluidics enables process intensification with laser induced cavitation and inertial ballistic
Presenter: David Fernandez Rivas (University of Twente)

Coffee Break

From 14:45 to 15:15, Forum (Ground floor)

Plenary lecture III & Poster Parade & Sponsor Pitch

From 15:15 to 17:00, Forum (Rabo Studio)

Chaired by: Andrea Ramírez Ramírez & Jun Yue

15:15 **[PL03] Title:** Year-round heat and CO_2 supply with combined hot water boiler and carbon capture technology
Presenter: Thomas Brouwe (HoSt)

16:00 **Poster parade & sponsor pitch**

Poster Session & Welcome Reception

From 17:00 to 18:30, Forum (Ground floor)

Conference Dinner

From 19:00 to 22:00, Forum (Rabo Studio)

Wednesday 9th of October 2024

Registration

From 8:30 to 9:00, Forum (Ground floor)

Announcements

From 9:00 to 9:15, Forum (Rabo Studio)

Plenary Lecture IV & Poster Parade

From 9:15 to 10:45, Forum (Rabo Studio)

Chaired by: Jun Yue & Jingxiu Xie

9:15 **[PL04] Title:** ISPT’s long term program process technology
Presenter: Sascha Kersten (University of Twente)

10:00 **Poster parade**

Coffee Break

From 10:45 to 11:15, Forum (Ground floor)

Parallel Session 3.1 Process System Engineering

From 11:15 to 12:30, Forum (NOK)

Chaired by: Mar Pérez-Fortes

11:15 **[KL05] Title:** Process Systems Engineering perspectives and new horizons
Presenter: Anton A. Kiss (Delft University of Technology)

11:45 **[OP33] Title:** Systematic evaluation and optimization of low-carbon technologies for Colombian oil refineries' decarbonization
Presenter: Erik López Basto (Delft University of Technology, Ecopetrol S.A.)

12:00 **[OP34] Title:** Energy and Exergy Analysis of a Coupled Dark Fermentation and Microbial Electrolysis Process for Sustainable Hydrogen Production
Presenter: Júlio Cesar de Carvalho Miranda (University of Twente)

12:15 **[OP35] Title:** Experimental investigation on the hydrodynamics of a conical bubbling fluidized bed with a novel gas distribution system
Presenter: Reddy Madhuri Manila (Delft University of Technology)

Parallel Session 3.2 (Bio)chemical Process Engineering

From 11:15 to 12:30, Forum (Camera 4)

Chaired by: Paolo P. Pescarmona

11:15 **[OP36] Title:** Photon flux and effective optical path length determination for continuous-flow photoreactor design through radiometry, chemical actinometry and ray-tracing
Presenter: Stefan Zondag (University of Amsterdam)

11:30 **[OP37] Title:** High yielding conversion of xylose to furfural via boronate esters
Presenter: Peter J. van der Wal (University of Twente)

11:45 **[OP38] Title:** Catalytic upgrading Kraft lignin pyrolysis bio-oil: effect of process parameters and sulfur content
Presenter: Matteo Borella (University of Genoa, University of Groningen)

12:00 **[OP39] Title:** Chemical recycling of HDPE and LDPE from municipal waste stream using Hydrothermal Liquefaction process
Presenter: Shih-Chieh Chien (University of Amsterdam)

12:15 **[OP40] Title:** The Interaction of Intrinsic Reaction and Mass Transfer in Polyethylene Pyrolysis with Reflux System
Presenter: Dwiputra M. Zairin (University of Twente)

Parallel Session 3.3 Electrochemical Engineering

From 11:15 to 12:30, Forum (Camera 1)

Chaired by: Ruud Kortlever

11:15 **[OP41] Title:** Optimizing electrochemical conversion of CO_2 to ethylene via multi-physics simulations
Presenter: Simone Dussi (TNO)

11:30 **[OP42] Title:** Regeneration of Iron Powder from Combusted Iron Products by Low-Temperature Electroreduction Method
Presenter: Akmal Irfan Majid (Eindhoven University of Technology, Universitas Gadjah Mada)

11:45 **[OP43] Title:** Salt accumulation in bipolar membranes reduces power in acid-base flow batteries
Presenter: Pavel Loktionov (Delft University of Technology)

12:00 **[OP44] Title:** Electro-separation technologies for sustainable chemical industry: technology ranking and industrial perspectives
Presenter: Michele Tedesco (TNO)

Parallel Session 3.4 Separation Technology & Transport Phenomena

From 11:15 to 12:30, Forum (Rabo Studio)

Chaired by: Kitty Nijmeijer

11:15 **[OP45] Title:** CO_2-Responsive Etalon Membranes (CREM) for in-situ analysis of ocean water
Presenter: Georgia Kontaxi (Delft University of Technology)

11:30 **[OP46] Title:** Development of novel polymeric precursors for the synthesis of selective carbon membranes for gas separation
Presenter: Clara Coiana (Eindhoven University of Technology)

11:45 **[OP47] Title:** Electrochemically mediated separation of carbon monoxide
Presenter: Christel Koopman (Delft University of Technology)

12:00 **[OP48] Title:** Advanced downstream processing for recovery of bioalcohols from fermentation broths
Presenter: Tamara Janković (Delft University of Technology)

12:15 **[OP49] Title:** Ferrofluidic millimeter-scale extraction systems for countercurrent slug flow liquid-liquid extraction
Presenter: Helda Niawanti (University of Twente)

Lunch Break & Poster Session

From 12:30 to 13:45, Forum (Ground floor)

Parallel Session 4.1 Renewable Carbon Conversion

From 13:45 to 15:00, Forum (NOK)

Chaired by: André Heeres

13:45 **[OP50] Title:** From waste to refinery – turning plastic waste into a suitable feedstock for the production of new materials
Presenter: Julian R.J. Strien (University of Groningen)

14:00 **[OP51] Title:** Induction heating with bulk inductive materials for reverse water gas shift reaction
Presenter: Liangyuan Wei (Eindhoven University of Technology)

14:15 **[OP52] Title:** Chemical recycling of hard to recycle mixed waste plastics
Presenter: Matthijs van Akker (BioBTX)

14:30 **[OP53] Title:** Waste plastic recycling: polypropylene hydrogenolysis over Ni/Al_2O_3 catalysts
Presenter: Xiyan Huang (University of Groningen)

Parallel Session 4.2 Reaction and Catalytic Engineering

From 13:45 to 15:00, Forum (Camera 4)

Chaired by: Sascha Kersten

13:45 **[KL06] Title:** Induction heating and direct Joule heating in intensified chemical processes
Presenter: Martin van Sint Annaland (Eindhoven University of Technology)

14:15 **[OP54] Title:** Batch and Continuous Degradation of Organic Pollutants in Water using Defect-Tuned Nanosized ZnO Photocatalysts
Presenter: Shuangxue Li (University of Groningen)

14:30 **[OP55] Title:** Light-assisted carbon dioxide reduction in an automated photoreactor system coupled to carbonylation chemistry
Presenter: Jasper H.A. Schuurmans (University of Amsterdam)

14:45 **[OP56] Title:** Pore Network Modeling of Hydrodynamics and Solute Dispersion in Packed Bed Reactors
Presenter: Ali Fathiganjehlou (Eindhoven University of Technology)

Parallel Session 4.3 Electrochemical Engineering

From 13:45 to 15:00, Forum (Camera 1)

Chaired by: Thijs de Groot

13:45 **[OP57] Title:** Hybrid water electrolysis: saving energy for the production of hydrogen
Presenter: Dulce M. Morales (University of Groningen)

14:00 **[OP58] Title:** Evaluating the role of A-site deficiency and exsolution of Ni-Fe nanoparticles in Sr2-xFe1.5-yMo0.5NiyO6±δ electrocatalysts for co-electrolysis of H_2O and CO_2
Presenter: Roelf Maring (University of Groningen)

14:15 **[OP59] Title:** Modification of perovskite oxide-based electrodes for efficient H_2 production in Protonic Ceramic Electrolyzers
Presenter: Nannan Li (University of Groningen)

14:30 **[OP60] Title:** Integration of in-situ water purification into zero-gap flow cell design for direct seawater electrolysis
Presenter: Ai-Yu Liou (Delft University of Technology)

Parallel Session 4.4 Separation Technology & Transport Phenomena

From 13:45 to 15:00, Forum (Rabo Studio)

Chaired by: Boelo Schuur

13:45 **[OP61] Title:** Towards Improving Negative CO_2 Emission: Optimizing Direct Air Capture Performance
Presenter: Amirreza Silani (Delft University of Technology)

14:00 **[OP62] Title:** Investigation of droplets captured by filter materials at the mesoscale in oil-gas separators
Presenter: Weiran Zhang (Eindhoven University of Technology)

14:15 **[OP63] Title:** Mass Transfer under Liquid-Liquid Slug Flow with Pickering Particles in Microreactors
Presenter: Tingting Wang (University of Groningen)

14:30 **[OP64] Title:** Dry fractionation of cohesive chickpea flour: impact of de-oiling and flow aids
Presenter: Koen Wetterauw (Wageningen University and Research)

14:45 **[OP65] Title:** Learning from Neural Networks: A Strategy to Identify Systematic Improvements to Activity Coefficient Models
Presenter: Daniël Emmery (Eindhoven University of Technology)

Coffee Break

From 15:00 to 15:30, Forum (Ground floor)

Plenary Lecture V & Awards & Closing Ceremony

From 15:30 to 17:00, Forum (Rabo Studio)

Chaired by: Peter Berben & Jun Yue

15:30 **Hoogewerff Gold Medal Ceremony**
[PL05] Title: Hoogewerff Gold Medal Lecture - Food Process Engineering, Engineering for Sustainability and Health
Presenter: Remko Boom (Wageningen University and Research)

16:30 **Awards & Closing Ceremony**

Tuesday 8th of October 2024

Poster Parade

From 16:00 to 17:00, Forum (Rabo Studio)

16:00 **[PP01] Title:** Accurate 2D & 3D Simulations of Eddy Currents for Targeted Heating via Induction Heating
Presenter: Frederik Nijkamp (Eindhoven University of Technology)

[PP03] Title: Selectivity control between Reverse Water-Gas Shift and Fischer-Tropsch Synthesis in Carbon-supported Iron-based Catalysts for CO_2 Hydrogenation
Presenter: Weixin Meng (University of Groningen)

[PP05] Title: Investigating deactivation and kinetics of levulinic acid hydrogenation on titania supported ruthenium catalysts
Presenter: Adarsh Patil (Eindhoven University of Technology)

[PP07] Title: Investing energy in hydrogen – accelerating applications of decentralised hydrogen
Presenter: Hans Gelten (Saxion University of Applied Science)

~~**[PP09] Title:** Pyrolytic Decomposition of Methane to Hydrogen and Functional Solid Carbon: Multi-Scale Modeling and Reactor Development~~
~~**Presenter:** David Reus (Eindhoven University of Technology)~~

[PP11] Title: Combined catalytic dehydrochlorination and pyrolysis for PVC waste stream
Presenter: Giulia Boccaccini (University of Groningen)

[PP13] Title: Modelling Aromatization in a Fluidized Bed Reactor
Presenter: Thirza Kuipers (Eindhoven University of Technology)

[PP15] Title: Aramazing – Chemical Recycling of Aramid Materials
Presenter: Dan Cristian Codita (University of Twente)

[PP17] Title: Process simulation of stepwise pyrolysis of cashew nut shell via Aspen Plus
Presenter: Chenyu Zhou (Eindhoven University of Technology)

[PP19] Title: A Closed Carbon Cycle Approach for Full Valorization of Lignocellulosic Biomass
Presenter: Amponsah P. Appiah (University of Groningen)

[PP21] Title: Minimizing ohmic resistance in alkaline water electrolyzers
Presenter: Saksham Pandey (Eindhoven University of Technology)

[PP23] Title: Electrochemical flow modelling of a semi-solid flow battery
Presenter: Simone Dussi (TNO)

~~**[PP25] Title:** Steady-state and dynamic modeling of a CO_2 electrolyzer: membrane electrode assembly~~
~~**Presenter:** Nasim Heydari (Delft University of Technology)~~

[PP27] Title: Gas holdup optimization in zero-gap alkaline water electrolysis via multiphase modelling
Presenter: Douwe Orij (Eindhoven University of Technology)

[PP29] Title: Alkaline water electrolysis beyond 3 A/cm^2
Presenter: Maximilian Demnitz (Eindhoven University of Technology)

[PP31] Title: Non-noble metal electrocatalysts for Hydrogen Evolution Reaction in PEM Water Electrolysis
Presenter: Bhavesh Chavan (Delft University of Technology)

[PP33] Title: Closed-Loop Recyclable Lignin-based Triboelectric Nanogenerators
Presenter: Yiwei Fan (University of Groningen)

[PP35] Title: Multifunctional Hydrogels for Underwater Motion Detection and Information Transmission
Presenter: Zeyu Zhang (University of Groningen)

[PP37] Title: Inverse gas chromatography, a new technique to investigate surfaces for porous media applications
Presenter: Maja Rücker (Eindhoven University of Technology)

[PP39] Title: Hydrogenation of bio-derived aldehydes over N-doped C-supported cobalt catalysts
Presenter: Ting Wang (University of Groningen)

[PP41] Title: Cs-enhanced Ru-based catalysts for low-temperature ammonia decomposition
Presenter: Gaetano Anello (Eindhoven University of Technology)

[PP43] Title: Methodology for Bubble Formation and Characterization in Viscous Media for Chemical Reactions
Presenter: Shivan Bissesar (University of Twente)

[PP45] Title: Isolation of anacardic acid from natural cashew nutshell liquid using ion exchange resins.
Presenter: Qian Zhou (Eindhoven University of Technology)

[PP47] Title: Electrical drying of biomass by electro-osmosis and electrohydrodynamic drying: effect of internal transport phenomena
Presenter: Aza Alawi (Delft University of Technology)

[PP49] Title: Thin-film-composite anion exchange membranes for increased OH-selectivity in CO_2-electrolysis
Presenter: Max Seling (Delft University of Technology)

[PP51] Title: Investigating the performance of commercially available nanofiltration membranes in alcohol-water mixtures at high pH
Presenter: Francisco Caparros-Salvador (University of Twente)

[PP53] Title: Numerical Investigation of bubble size effect on the gas hold-up in a constant gas flow rate
Presenter: Mehrshad Rezadoost Dezfuli (Eindhoven University of Technology)

[PP55] Title: Development and Validation of an In-House CFD Code for Slurry Bubble Columns
Presenter: Sriram Ramanathan (Eindhoven University of Technology)

[PP57] Title: Energy and Exergy Analysis of a Coupled Dark Fermentation and Microbial Electrolysis Process for Sustainable Hydrogen Production
Presenter: Júlio Cesar de Carvalho Miranda (University of Twente)

[PP59] Title: Resin beads as metal-free catalysts for the synthesis of cyclic carbonates
Presenter: Jing Chen (University of Groningen)

Wednesday 9th of October 2024

Poster Parade

From 10:00 to 10:45, Forum (Rabo Studio)

10:00 **[PP02] Title:** Modelling framework for Direct Air Capture process: Investigating CO_2-H_2O co-adsorption on amine functionalized sorbents
Presenter: Mattia Galanti (Eindhoven University of Technology)

[PP04] Title: Syngas Production by Plasma-Assisted Decomposition of $KHCO_3$ in an Integrated Carbon Capture and Utilization Process
Presenter: Huub van den Bogaard (University of Groningen)

[PP06] Title: Methanol synthesis from CO_2 using a co-precipitated ZnO/ZrO_2 catalyst in a continuous spinning basket reactor
Presenter: Mochamad Firmansyah (University of Groningen)

[PP08] Title: The Utilization of Humin Ozonolysis Product via Bioconversion using Oleaginous Yeast
Presenter: Khairul Hadi Burhan (University of Groningen)

[PP10] Title: Taking off with Furfural: The missing link in the production of high performance jet fuel
Presenter: Rick Baldenhofer (University of Twente)

[PP12] Title: Coupling Mild Flow-through Organosolv Extraction and Catalytic Oxidation from Lignocellulosic Biomass with High S-type Units towards Benzoquinones
Presenter: Ge Guo (University of Groningen)

[PP14] Title: 1D model of droplet drying using interface receding approach
Presenter: Sanaz Aghaei (Eindhoven University of Technology)

[PP16] Title: Cooperative integration of thermal solar and wind energy with molten salts and green ammonia enables sustainable power generation in Morocco
Presenter: Yori Foppen (University of Twente)

[PP18] Title: Techno-economic analysis of circular plastic production using induction heating
Presenter: Melany Gomez Arciniegas (Eindhoven University of Technology)

[PP20] Title: Mitigating Hydrogen Crossover in Alkaline Water Electrolysis (AWE)
Presenter: Jelle Prinsen (Eindhoven University of Technology)

[PP22] Title: PyDOLPHYN: Dynamic modelling for optimal system integration of water electrolysis
Presenter: Simone Dussi (TNO)

[PP24] Title: Indirect CO_2 capture: extracting CO_2 from concentrated seawater using bipolar membrane electrodialysis
Presenter: Vojtech Konderla (Delft University of Technology)

[PP26] Title: Scalable fabrication of catalysts for proton exchange membrane water electrolysis
Presenter: Bhavesh Chavan (Delft University of Technology)

[PP28] Title: Nanostructuring Ni-based porous transport layers for anion exchange membrane water electrolysis
Presenter: Ameya Ranade (DIFFER)

[PP30] Title: Atomic Layer Deposition for Proton-Exchange Membrane Water Electrolysis
Presenter: Athina Tzavara Roussi (Delft University of Technology)

[PP32] Title: Gravity-Fed Laminar Electrolyser
Presenter: Vincent Botond Polet (Delft University of Technology)

[PP34] Title: Unentangling PVC recycling: Challenges, Gaps, and Perspective
Presenter: Martijn Meijer (University of Groningen)

[PP36] Title: Design and development of bio-based amphiphilic polymers with antibacterial properties
Presenter: Zao Cheng (University of Groningen)

[PP38] Title: Experimental characterization of co-adsorption kinetics and thermodynamics in solid sorbents for DAC
Presenter: Timothy van Lanen (Eindhoven University of Technology)

[PP40] Title: Effect of molecular weight on transport limitation in Plastic Hydrogenolysis
Presenter: Preethi Venugopal (University of Twente)

[PP42] Title: Catalytic conversion of lower olefins to BTX range of aromatics using zeolite-based catalysts
Presenter: Paresh Butolia (University of Groningen)

[PP44] Title: Electrodialysis Based Membrane Assisted Electro-Osmotic Dewatering of Biomass
Presenter: Selvaraj Chinnathambi (University of Groningen)

[PP46] Title: Modelling CO_2 adsorption for Direct Air Capture using Multiphysics CFD
Presenter: Sebastiaan Kuipers (Delft University of Technology)

[PP48] Title: Development of porous carbon materials for methane capture from diluted streams
Presenter: Giulia De Felice (Eindhoven University of Technology)

[PP50] Title: Bio-based Solvents for Circular Poly Vinyl Chloride Processing
Presenter: Farzaneh Ghazizadeh Ahsaie (University of Twente)

[PP52] Title: Design and scale-up of membrane reactor for ammonia synthesis
Presenter: Iolanda Gargiulo (Eindhoven University of Technology)

[PP54] Title: Eulerian-Lagrangian Simulation of Bubble-Liquid Interphase Mass Transfer in a Slurry Bubble Column
Presenter: Majid Mansouri Borujeni (Eindhoven University of Technology)

[PP56] Title: A Simplified Analytical Model for the Impurity Heating Hypothesis of Laser-Induced Crystal Nucleation
Presenter: Pepijn van Tooren (Delft University of Technology)

[PP58] Title: Design of a separation system for the closed-loop superheated steam drying process in the paper industry
Presenter: Felipe Oliveira (University of Twente)

Author: Tom van Aken (Avantium, The Netherlands)

Title: **[PL01]** The long road of scaling renewable chemical process technology. The Avantium story on how to bring the new, plant-based polyester PEF to market

CV:

Tom van Aken has studied Chemistry at the Utrecht University. He started his career in the chemical industry at DSM, working for their fine chemicals division in Europe and the United States. In 2002 he joined the start-up company Avantium, where he became CEO in 2005. Under his leadership, Avantium has grown into a world leader in renewable chemistry technologies, focusing on new plant-based polyesters. Avantium is a listed company at the Euronext Stock exchange since 2017. Tom lives in Haarlem, The Netherlands, and is father of 3 daughters. Since 2019 he is member of the Topteam Chemistry.NL and he is the chair of the Dutch start-up roundtable for companies in the chemicals and materials sector.

Author: Raffaella Ocone (Heriot-Watt University, UK)

Title: **[PL02]** From Applications to Fundamentals: The Power of Multiscale Modelling

CV:

Raffaella Ocone OBE, FREng, FRSE holds degrees from the Università di Napoli, Italy, and Princeton University, USA. She holds the Chair of Chemical Engineering at Heriot-Watt University, UK, and is a Guest Professor at Ruhr University Bochum, Germany. Currently, she serves as the Deputy President of the Institution of Chemical Engineers (IChemE) and will become the 84th President in 2025. In 2007, Raffaella was honoured with the title of Cavaliere by the President of the Italian Republic. In 2019, she was recognised as one of the top 100 Most Influential Women in the Engineering Sector by Inclusive Boards, in partnership with the Financial Times. In 2017, she became the inaugural "Caroline Herschel Visiting Professor" in Engineering at Ruhr University Bochum, Germany, in recognition of her contributions to engineering ethics. affaella's research primarily focuses on modelling multiphase reactive systems, with a particular emphasis on developing responsible technologies in the energy sector. Her current work centres on advancing low-carbon hydrogen production.

Abstract:

Engineers frequently use macroscopic models to facilitate the design, development and operation of equipment, technologies and processes. While these models are often considered “predictive”, they typically provide only qualitative insights and trends. Accurate quantitative predictions are less common, particularly for complex systems and processes. This limitation arises from challenges such as the lack of effective methodologies to scale up microscopic physics, the inability to accurately describe mesoscale phenomena and the absence of appropriate constitutive equations.

In the context of particulate flow, existing models and theories often fall short in terms of robustness, predictability and flexibility, making it difficult to fully capture the range of behaviours observed in these systems. Industrial issues like particle agglomeration are still managed largely through empirical methods and ad-hoc models tailored to specific flow conditions, relying heavily on operator expertise.

This presentation will focus on one of the models used for granular and particle laden flows, namely the kinetic theory for granular flow (KTGF), which draws an analogy between solid particles and gas molecules to effectively model the macroscopic behaviour of particulate flow. Despite its successes, KTGF has shown limitations that will be discussed, along with the challenges it presents. Our ongoing research in this area will also be highlighted and critically assessed.

Author: Thomas Brouwe (HoSt, The Netherlands)

Title: **[PL03]** Year-round heat and CO_2 supply with combined hot water boiler and carbon capture technology

CV:

Dr. Ir. Thomas Brouwer, born in Deventer, studied Chemical Engineering at the University of Twente from 2009 to 2015, including a board year at C.T.S.G. Alembic. During his studies, he met his wife, and he is now a proud father of a beautiful daughter. He continued pursuing a PhD in solvent-based affinity separation under Boelo Schuur and Sascha Kersten at the Sustainable Process Technology Group at the University of Twente. Alongside his PhD, he served as a part-time lecturer, teaching courses such as Physical Transport Phenomena and Chemical Process Design. After completing his PhD, Thomas began working as an R&D Engineer at the HoSt Group, specializing in gas purification and separation technologies for biogas, flue gas, and landfill gas. Currently, as a product manager at Bright Renewables, a subsidiary of HoSt Group, he focuses on developing modular carbon capture systems while continuing research on long-term technological innovations within the HoSt Group.

Abstract:

HoSt Group is a leading international company specializing in the design, construction, and maintenance of renewable energy systems. Established in 1991 and headquartered in Enschede (NL), the company focuses on bioenergy solutions such as biogas plants, biomass thermal systems, hydrogen systems and waste-to-energy systems. HoSt aims to accelerate the transition to sustainable energy by developing in-house cutting-edge technologies for the conversion of organic waste into renewable energy (electricity, steam, biomethane) and other useful products such as food grade liquid CO_2 , (bio)hydrogen, renewable fertilizers. With a strong commitment to innovation and environmental sustainability, HoSt serves clients globally, including municipalities, industries, and agricultural sectors. In this talk, we will showcase a unique real-world project where several of these technologies are combined to provide year-round heat and CO_2 to over 25 hectares of greenhouses. This project addresses not only the technical and operational aspects but also considers seasonal and day/night variations, crop growth cycles, and both planned and unplanned maintenance stops. It serves as an excellent example of engineering in the sustainable technology field.

Author: Sascha Kersten (University of Twente, The Netherlands)

Title: **[PL04]** ISPT's long term program process technology

CV:

Sascha Kersten obtained his MSc degree in chemical engineering from the University of Amsterdam, and a PhD on biomass gasification in circulating fluidized beds from the University of Twente. He started his career at the Energy Research Centre of the Netherlands, where he worked on modeling of dynamic systems and later on biomass conversions. Since 2003 he has been working at the University of Twente. There, Sascha was appointed full professor in Sustainable Process Technology in 2011. Since 2018 he is associated with ISPT, the Institute for Sustainable Process Technology. He is chairman of the Academic Advisory Board and Program Director of the Long Term Program since 2023.

Abstract:

The Long Term Program (LTP) is an ambitious initiative by the Institute for Sustainable Process Technology aimed at developing process technology for 2050. By then, the value chains from raw materials to end products in industry are expected to have changed radically. Unique to the Netherlands, the LTP focuses on pioneering technologies that do not yet exist today, setting the stage for a fully sustainable process industry. The LTP program brings together scientists from socio-economic transitions, (bio)process technology, catalysis and materials technology, and partners them with companies in chemistry, materials, energy production and food. This interdisciplinary and cross-technology approach is essential for the actual implementation of innovations. During NPS 19, Sascha will explain more about LTP and the first projects that have started within the program: TREPS (Trace Removal Using Electrically Powered Separations) and SUNSOLr: Electrification of Chemical Conversions.

Author: Remko Boom (Wageningen University and Research, The Netherlands)

Title: **[PL05]** Hoogewerff Gold Medal Lecture - Food Process Engineering, Engineering for Sustainability and Health

Abstract:

The food industry has steadily become more prominent in The Netherlands and Europe, and has become the country's largest industrial sector with a total production value of 91.2 billion euro in 2022. As a trading nation, processing raw materials into higher value ingredients and foods is crucial, and therefore, food process engineering is crucial for our future.

The technology for processing foods faces several challenges. It directly impacts the quality and taste of the foods that we all eat, and therefore also creates emotion with consumers, to which the technology has to answer. At the same time, global food production is one of the main contributors to the emissions of greenhouse gases, while the availability of sufficient, high quality food will be a prime challenge in the coming decades due to climate change related land degradation and growth of the global population. The technology that we currently use for the conversion of the raw materials that we produce on agricultural land, into edible foods, is not very efficient. Only a relatively small part of the total amount of protein that is grown on the land, reaches our plates. This is due to losses over the chain, but also because our current technology for creating food ingredients from their raw materials has often relatively low yield and requires significant amounts of water, chemicals and energy.

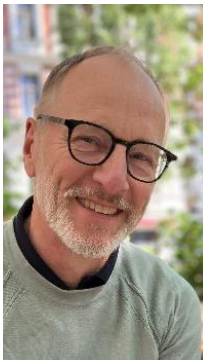
This can improve if we change our perspective on what food processing should achieve. Traditionally, chemical engineering investigates methods to produce pure, well-defined chemicals and materials. But foods are by nature almost never pure, and generally have an intricate microstructure that is quite important for its properties. We have worked already for many years on developing 'gentle' processing methods that reduce the degree of refining and aim for the right properties instead of high purity. With the ingredients that come from this technology, one can create well-structured and stable foods, that could also have better nutritional value. At the same time, the raw material are better utilized, leading to less side streams with higher quality. This new generation of gentle processing methods is becoming accepted by the sector and will allow us to create more high-value foods from less raw materials, that fit in a healthier diet, and will result in significantly less waste throughout the chain.

Keynote

Author: Hans Lammers (Nobian Industrial Chemicals B.V., The Netherlands)

Title: **[KL01]** Membrane electrolysis: essential for chemicals; enabler for sustainable process and product development

CV:



Mr. Hans Lammers is Senior R&D expert Electrolysis and Membranes at Nobian Industrial Chemicals B.V. After his Bachelor Analytical Chemistry and Master Chemistry (University Utrecht), he continued his career at AkzoNobel in various R&D roles including Specialist in electrochemical membrane processes and R&D team leader membrane technology. In 2018, AkzoNobel separated Chemicals to become Nouryon and in 2021, Industrial Chemicals separated to become Nobian. At that point, Hans got closer connected to Chlor Alkali industrial operations and electrolysis technology suppliers. Currently, Hans works in Nobian R&D mainly on membrane electrolysis to support the Circular and Renewable agenda of Nobian with focus area on closing salt loops and the development of battery chemicals and their processes. The latter involves a cooperation project on Fundamentals of Chlor Alkali electrolysis with Eindhoven University (Dr. Thijs de Groot)

Abstract:

Membrane electrolysis of salt brine is an essential process for the production of caustic, hydrogen and chlorine. The latter is an important chemical in everyday life and a major building block for the chemical and pharmaceutical industries. Some 55% of European chemical production relies on this process and many chemicals, plastics and medicines depend on chlorine during the manufacturing process. The core technology is about electrochemistry and membranes and together with suppliers, knowledge institutes, and other partners we continuously strive to reduce energy consumption of this energy intensive yet, very energy efficient process. In this presentation, I will share some of our experiences, its challenges and the opportunities to develop membrane electrolysis processes for creating new products and closing loops in chemical manufacturing.

Author: Francesco Picchioni (University of Groningen, The Netherlands)

Title: **[KL02]** Design of sustainable polymeric products

CV:

Francesco Picchioni, born in Italy in 1971, got his MSc (1996) and PhD (2000) degrees from the University of Pisa in Italy for works related to polymer blends, functionalization under the supervision of Prof. F. Ciardelli. After a postdoctoral position (2000-2002) at the Eindhoven University of Technology (TU/e), he joined the University of Groningen first as assistant- (2003-2008), then associate- (2008-2013) and full professor (2014-present). He is currently the chair of the Product Technology group. His research interests include polymer modification and blending with focus on novel materials for the circular economy.

Abstract:

The societal ambition to become circular (in the Netherlands in 2050) has prompted in the last few decades many research activities aimed at providing solutions for polymer recycling. In this work, we will start by presenting some of our own work related to the design for recycling polymers. In particular, we will provide an extensive overview of our work on covalently adaptable network (CAN) as conceptual tool for the recycling of rubbers and thermosets. Many novel materials based on this concept will be illustrated in terms of their preparation, thermal and mechanical behaviour before and after recycling. Subsequently, we will present some of our recent work focused on currently commercialized materials including rubbers, poly(vinyl chloride) and polyolefins. The current status of the corresponding technologies will be discussed and a few examples will be provided of polymeric products based on a substantial percentage of recycled materials.

Author: Peter de Jong (ISPT, The Netherlands)

Title: **[KL03]** Without process innovation no protein transition

CV:

Peter de Jong is a chemical engineer by training and received his PhD degree at the Delft University of Technology. His professional career started with FrieslandCampina in 1986. In 1987, he joined NIZO food research and became a leading expert on optimization of international dairy/food processing with respect to product quality, costs and sustainability using computer simulation tools. In 2013 he became program director at the Institute of Sustainable Process Technology (ISPT), focusing on development of new technology (e.g. mild fractionation, drying) with consortia of large food companies. In 2014, he received a professorship in Dairy Process Technology at VHL University in Leeuwarden. At NIZO food research he is still active as a principal scientist on food processing. In 2021, he was appointed as program director of the so-called “Fascinating” national program, an open innovation program for realization of a circular agri-food system in the province of Groningen. Peter has an extensive network in the dairy industry and initiates new research projects to enhance the food production chain every year. Peter published 200+ scientific and technological papers and 100+ industrial reports.

Author: David Fernandez Rivas (University of Twente, The Netherlands)

Title: **[KL04]** Microfluidics enables process intensification with laser induced cavitation and inertial ballistic

CV:

David Fernandez Rivas obtained his PhD at the University of Twente UT (2012). Assistant professor (2014-2019), associate professor (2020-2021) and Professor (2021) in the Mesoscale Chemical Systems Group, UT. David’s research interest and expertise are in the areas of microfluidics, transdermal drug delivery alternatives, solar-to-fuel cells, process intensification, acoustic cavitation and sonochemistry. In 2019, he obtained the European Research Council Starting Grant for his project BuBble Gun, aimed at penetrating microjets in soft substrates, towards controlled needle-free injections. David received the prestigious VIDI grant, from the Dutch Research Council in 2023. He has received several recognitions, such as the Young Sonochemist Award, given by the Japan Society of Sonochemistry (JSS) in 2011, the Pieter Langerhuizen Lambertuszoon Fonds prize (2016) awarded by the Royal Holland Society of Sciences and Humanities (KHMW), and elected as Engineer of the Year 2021, and the Prince Friso Award by the Royal Dutch Institute of Engineers (KIVI). His work in Public Outreach earned him the Stairways to Impact Award, granted by the Dutch Scientific Council, and the UT in the Media Award, both in 2021. He was elected to the Global Young Academy (2020) and the Young Academy Europe (2020), elected Secretary in 2023. In 2024, David was installed at the De Jonge Akademie (Dutch Young Academy), Royal Netherlands Academy of Arts and Sciences. David has co-authored over 60 reviewed journal papers and wrote the book Empathic Entrepreneurial Engineering. He is inventor of a patent commercialized by the spin-off BuBclean (2013) of which he is cofounder. He also founded FlowBeams, a spin-off from the University of Twente (2021) to valorize his research and second patent on needle-free injections. He was co-chair of the COST Action Greenering: Green Chemical Engineering Network towards upscaling sustainable processes, from the European Cooperation in Science & Technology (2019-2022). He also serves in the editorial board of several journals, such as Ultrasonics Sonochemistry, and Biomicrofluidics.

Abstract:

In the last decade, Process Intensification through microfluidics has proven its advantages in Chemical Engineering, with clear benefits when aiming for more sustainable and efficient ways to operate chemical processes. A growing number of companies have demonstrated that “large” equipment is not necessarily the only way to reach an economy of scale, and chemical engineers are more comfortable with scaling-down strategies. Our team has developed the BuBble Gun microfluidics platform to accelerate small liquid volumes with utilization potential in biomedical applications. We are now developing new experiments to demonstrate the technological potential in novel process designs and chemical reactions. This platform can be used to control physicochemical phenomena at the microscale with droplets and bubbles along three testing frameworks: 1) Cavitation: where we have promising results showing the manipulation of ultrafast contact line dynamics, e.g., coating the inner walls of microfluidic channels with gold. 2) Jetting: The channel geometry and coatings influence the jet breakup, the resulting drop size distribution, and the jet trajectory. The jets are inertia dominated and

we study viscoelastic effects with different additives. 3) Impact: We have numerical and experimental studies of the fluid dynamics. Our approach offers advantages for manipulating viscous forces, surface tension, and mass transport, which are concomitant factors when dealing with chemical engineering concepts.

Author: Anton A. Kiss (Delft University of Technology, The Netherlands)

Title: **[KL05]** Process Systems Engineering perspectives and new horizons

CV:

Tony Kiss is a professor of chemical engineering at Delft University of Technology, and a visiting professor at University of Manchester. He is a Fellow of IChemE and Royal Academy of Engineering, with over 25 years of academic and industrial experience. He worked for over a decade as a Senior Project Manager and RD&I Specialist at AkzoNobel Chemicals. Besides his key industrial role, he was also appointed as part-time professor at University of Twente. During the past decade, he carried out many research & industrial projects, supervised graduation projects, published over 25 textbooks, book chapters, and 100+ scientific articles in highly-ranked journals. For his pioneering research, he received the Royal Society Wolfson Research Merit Award for outstanding scientists, Recent Innovative Contribution in CAPE award for outstanding innovative contributions to recent advances in CAPE ideas, methods and/or tools, Hoogewerff Jongerenprijs (a very prestigious award recognizing the most promising young scientist in The Netherlands), the AkzoNobel Innovation Excellence Award (for the most successful industrial innovation), Pirkey Distinguished Lecturer in Chemical Engineering (University of Texas at Austin, USA), and CHEMCON Distinguished Speaker Award for innovators and science leaders (IIChE, New Delhi, India).

Abstract:

Process Systems Engineering (PSE) deals with methods and tools to support decision-making for the creation and operation of chemical supply chains, including the discovery, design, manufacturing, processing, and distribution of chemical products. In other words, PSE is about educated decision-making, at all levels and (size/time) scales, by understanding complex systems using a holistic view. This lecture aims to provide an informative industrial and academic perspective on PSE, from a personal viewpoint of the author – a seasoned professional with more than 25 years of combined industrial and academic experience. The main topics covered include: PSE in academic education vs industrial needs, PSE research vs industrial projects, personal perspectives, lessons learned in industry, global challenges and trends, professional skills, opportunities and new horizons for PSE.

Author: Martin van Sint Annaland (Eindhoven University of Technology, The Netherlands)

Title: **[KL06]** Induction heating and direct Joule heating in intensified chemical processes

CV:

After earning his PhD in Chemical Engineering at the University of Twente in 2000, van Sint Annaland joined the Fundamentals of Chemical Reaction Engineering research group there, starting as an Assistant Professor and later becoming an Associate Professor. In 2010, he became a Full Professor at Eindhoven University of Technology, heading the Chemical Process Intensification research group. In 2020, he also became the Scientific Director of the post-master's course in Process and Product Design at the same university. His research focuses on developing innovative multi-functional reactors using advanced, experimentally validated models. Key areas include integrating reaction and separation processes (e.g., membrane reactors, chemical looping, and sorption-enhanced processes), dynamic heat exchange in reactors, and electrifying chemical reactors, particularly via methods like direct Joule heating and inductive heating.

Abstract:

Induction heating and direct Joule heating are advanced thermal techniques that enable the electrification of chemical industries, helping to reduce anthropogenic CO_2 emissions by replacing fossil fuel combustion with renewable energy sources for heating. These methods hold promise for application in chemical processes to enhance overall energy efficiency and ensure precise temperature control. Induction heating uses electromagnetic fields to generate heat within inductive materials, allowing for rapid and efficient heating, which is essential for high-temperature reactions and processes requiring controlled environments. Joule heating, also known as resistive heating, generates heat by passing an electric current through a conductor or semiconductor. This technique can be used for direct heating of both conductive and non-conductive materials when combined with (semi-)conductive additives. In chemical reaction engineering, these heating methods support efficient catalytic processes, enable continuous flow reactors, and optimize energy use. They also offer scalability and automation potential, meeting industrial demands for sustainable and cost-effective chemical production. The integration of these heating techniques into chemical reactors represents a significant advancement toward electrified chemical engineering processes, such as CO_2 capture, reverse water gas shift, methane reforming, and biomass and plastic pyrolysis. In this presentation, we will highlight our modelling and experimental studies in this field.

Author: Adarsh Patil (Eindhoven University of Technology)
Other Authors: Afnan Ahmad, Eindhoven University of Technology; M.F. Neira d'Angelo, Eindhoven University of Technology

Title: **[OP01]** Biphasic furfural synthesis from biorefinery feed using coated 3D foam structures

Abstract: Furfural stands out as an important bio-oxygenate to substitute fossil derived chemicals [1]. Its synthesis from hemicellulose (C5 sugars) has been done using homogeneous acids such as H_2SO_4 and HCl since 1941 [2]. Heterogeneous catalysts are an attractive alternative to minimize corrosion and easier downstream separation. Regardless, furfural yields still remain <50% in monophasic (aqueous only) conditions. Recently, biphasic systems combining the use of a hydrophobic organic solvent and the reacting aqueous medium have resulted in increased furfural yields (70-80%) using both homogeneous and heterogeneous catalysts [3,4]. These demonstrations were done in batch and micro/millireactors, limited by volume and numbering up, respectively, to achieve high throughput. Therefore, we present scalable, catalyst coated 3D foam structures facilitating lower pressure drop and fast transport to obtain high furfural yields in a continuously operated system. Coated foams (1 cm diameter and 2 cm long) of required catalyst mass prepared by dip coating method were packed in the reactor (1 cm i.d. *10 cm length) in a downflow configuration, and samples taken at regular intervals. Analysis of the aqueous and organic samples were done using HPLC and GC, respectively. Benefits for increased furfural yields are observed at xylose conversion > 80-85% for 3D foam structures using real biorefinery feed rich in C5 and C6 sugars, compared to batch operation using xylose as model feed. While using toluene as the organic solvent, a significant increase in pressure drop was observed across the reactor at high temperatures (180 and 190°C), indicating severe formation of humins that deposit on the catalytic structure. Substituting toluene with sec-butylphenol (SBP) leads to stable operation with minimal pressure drop. SBP co-extracts both furanic compounds, thus minimizing the formation of polymeric species. An activation energy of 96 $kJ\cdot mol^{-1}$ was observed for coated foam catalysts similar to that for powder catalyst tested n batch autoclaves indicating the absence of either external or internal mass transfer limitations. Stable activity with coated foams up to 36 hours was demonstrated with a low organic solvent to aqueous ratio (2:1 vol.). Competitive furfural productivity of $5.85\cdot10^{-2}$ $g_{furfural}g_{cat}^{-1}min^{-1}$ was observed, at least 25 times higher than the previously highest reported value in literature using real biorefinery feed. Therefore, these coated structures present an attractive and scalable alternative for the solid-catalyzed production of furfural in future biorefineries.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N°101006618. The present publication reflects only the author's views and the European Union is not liable for any use that may be made of the information contained therein.

References
[1] Werpy, T, Petersen, G., Eds.; U.S. Department of Energy (DOE), 2004. Top Value Added Chemicals from Biomass Vol. I.
[2] Dunlop, A. P. Ind. Eng. Chem. 1948, 40, 204–209.
[3] M Papaioannou, et al., Ind. Eng. Chem. Res. 2019 58 (35), 16106-16115.
[4] C. Aellig et al., Catal. Sci. Technol., 2015,5, 142-149.

Author: Chencong Ruan (University of Groningen)
Other Authors: Hero Jan Heeres, University of Groningen; Jun Yue, University of Groningen

Title: **[OP02]** Transformation of glucose to 5-hydroxymethylfurfural over $AlCl_3$ catalyst in water: the effect of choline chloride addition

Abstract: The use of sustainable resources such as lignocellulosic biomass as the feedstock is considered as a promising way to reduce the reliance on the conventional fossil fuels. The catalytical transformation of biomass-derived carbohydrates to 5-hydroxymethylfurfural (HMF) has received increasing attention, because HMF as a platform compound can be used to produce a variety of chemicals, biofuels and biopolymer building blocks [1]. HMF is typically produced in water via the dehydration of hexoses (generally glucose) over homogenous/heterogeneous Brønsted and/or Lewis acids [2]. The degradation of glucose and HMF to humins significantly reduces the carbon balance and HMF selectivity. Accordingly, strategies such as biphasic solvent system and halide promoter (e.g., NaCl) are used to improve the HMF synthesis [3].

In this work, the conversion of glucose to HMF was conducted in aqueous ChCl solution over homogeneous $AlCl_3$ catalyst. The initial experiments were conducted in the monophasic aqueous system at 140 oC, where a maximum HMF yield of ca. 45% was obtained. The formation of glucose isomers, fructose and mannose, was observed. Their yields showed a clear maximum in the initial stage, indicating that they are intermediates and prone to further HMF synthesis. The experiments using fructose or mannose as the substrate were also performed, both of which demonstrated a higher reactivity towards HMF. Similar to the case of glucose conversion, the presence of these three sugars was found in the reaction solution, showing that there are reversible conversions between glucose, fructose and mannose. The addition of ChCl significantly enhanced the conversion rate of hexoses and HMF selectivity. Based on these results and our previous work [3], the reaction network for glucose transformation to HMF in aqueous ChCl solution was proposed. In order to obtain deep insights into the reaction network, a comprehensive kinetic model was developed, based on the monophasic experiments in a range of temperatures (100-160 ℃), initial concentrations of sugars (glucose, fructose or mannose, 0.2-0.9 M), HMF (0.2-0.9 M) and ChCl (1.8-4.6 M). The kinetic parameters for each sub-reaction and the effect of ChCl on the reaction chemistry were elucidated based on the model. Furthermore, the kinetic model allowed to predict the optimum reaction conditions, according to which the HMF synthesis from glucose was performed under biphasic operation using methyl isobutyl ketone as the extraction solvent and an HMF yield of ca. 65% could be obtained.

References

[1] R. van Putten et al., Chem. Rev., 2013, 113(3), 1499-597.
[2] Q. Hou et al., Green. Chem., 2021, 23(1), 119-231.
[3] W. Guo et al., Chem. Eng. J., 2020, 381, 122754.

Author: Hans Gelten (Saxion University of Applied Science)
Other Authors: Benno Aalderink, Saxion University of Applied Science; Hossein Nami, Syddansk Universitet; Bert Heesink, Demcon Suster; Wim de Jong, Twence; Richard van Leeuwen, Saxion University of Applied Science

Title: **[OP03]** Power-to-Methanol: techno-economical evaluation of a digestion use-case

Abstract: An important future sustainable raw material for the process industry is green hydrogen, produced via electrolysis of water with solar- or wind energy. For hydrogen, there are several important promising applications, i) as a fuel for high-temperature processes or ii) as an energy carrier for fuel cell technology (e.g. transport sector). Another promising applications is as a raw material for the production of sustainable bulk chemicals such as methanol (MeOH). Worldwide MeOH consumption is expected to rise ~40 % till 2035 (Ouda et al. 2016). At the Twence biodigestion plant in the east of The Netherlands, there are plans for production of green MeOH using captured CO_2. This plant has the potential to produce up to 10 tonnes of MeOH each hour. However, to result in a good business case, a thorough and specific analysis of all the production steps in this use-case is required.

The concept of Power-to-X (PtX) was first published in 2013, with Power-to-Gas being the first alternative to be discussed. The term has evolved from Power-to-Gas to the broader approach of Power-to-X, including Power-to-MeOH.

Several pilot-studies in literature mention that the involved processes in green MeOH are economically not viable at present time. The production costs of green MeOH is much higher then using a conventional method, due to the high costs of renewable energy to produce green hydrogen (up to 60-70 % share in the cost price) (Ouda et al. 2016, Pratschner et al. 2023). However, there are clearly large variations in the cost price of MeOH production from one use-case to another, ranging from 530 to 2706 €/tonne MeOH and no clear insights on the cause of these variations and the gap between sustainable and fossil-based MeOH.

The presented work focusses on the techno-economic assessment (TEA) (Nami et al. 2024) of green-methanol production via carbon capture for the situation at the Twence site. For different scenarios the required fixed capital investment (CAPEX), operational expenditure (OPEX) and potential revenue are calculated and predicted considering near-future trends and expectations.

References

[1] Nami, H., Hendriksen, P. V., & Frandsen, H. L. (2024). Green ammonia production using current and emerging electrolysis technologies. Renewable and Sustainable Energy Reviews, 199, 114517.

[2] Ouda, M., Hank, C., Nestler, F., Hadrich, M., Full, J., Schaadt, A., & Hebling, C. (2019). Power-to-Methanol: Techno-Economical and Ecological Insights. In W. Maus (Red.), Zukünftige Kraftstoffe (pp. 380-409). Springer Berlin Heidelberg.

[3] Pratschner, S., Radosits, F., Ajanovic, A., & Winter, F. (2023). Techno-economic assessment of a power-to-green methanol plant. Journal of CO2 Utilization, 75, 102563.

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Title: **[OP04]** Synthetic kerosene from CO_2-rich synthesis gas via Fischer-Tropsch synthesis

Abstract: Carbon capture and conversion into aviation fuel range hydrocarbons is an appealing technology considering the large energy demand of the aviation sector and the few available Alternatives [1]. The conversion of CO into long chain hydrocarbons via Fischer Tropsch synthesis (FTS) over cobalt-based catalysts has been extensively investigated, but the conversion of CO_2 over these catalysts produces mainly methane [2]. Therefore CO_2 requires conversion into CO via the Reverse Water Gas Shift (RWGS) which is an endothermic equilibrium reaction. As the CO_2 equilibrium conversion is around 40-60% at industrial relevant conditions (Fig. 1A), the need for a CO_2 separation step to suppress methanation is evident. However, if the Fischer Tropsch process would be tolerant for CO_2, an intensive CO_2 separation step can be avoided.

The performance of cobalt-based catalysts for $CO_2/CO/H_2$ mixed feed is debated as some researchers claim that CO_2 is an inert whereas others claim that CO_2 is partly hydrogenated into methane [3-5]. To rule out conversion effects on selectivity, the influence of CO conversion on C_{5+} selectivity under a mixed feed of 50% $CO_2/(CO+CO_2)$ is investigated (Fig. 1B). C_{5+}-selectivity is found to be stable at 80 % in the full range of CO conversion evaluated (15-80 %). In Fig. 1C the influence of CO_2 content in the feed on the selectivity is presented. The selectivity to C_{5+}-hydrocarbons of mixed feeds up to 75% CO_2 remains at least 80 % but at higher CO_2 concentration, the C_{5+}-selectivity decreases. However, CO_2 conversion is negligible which suggests that other causes are responsible for the decrease in selectivity rather than CO_2 methanation. Based on these results, the possible CO_2-concentration in a mixed feed Fischer-Tropsch process for the efficient production of synthetic aviation fuels is determined. In this contribution, it will be established under which conditions CO_2 can be regarded as an inert and the precise causes behind the loss of C_{5+}-selectivity at high CO_2 content will be discussed.

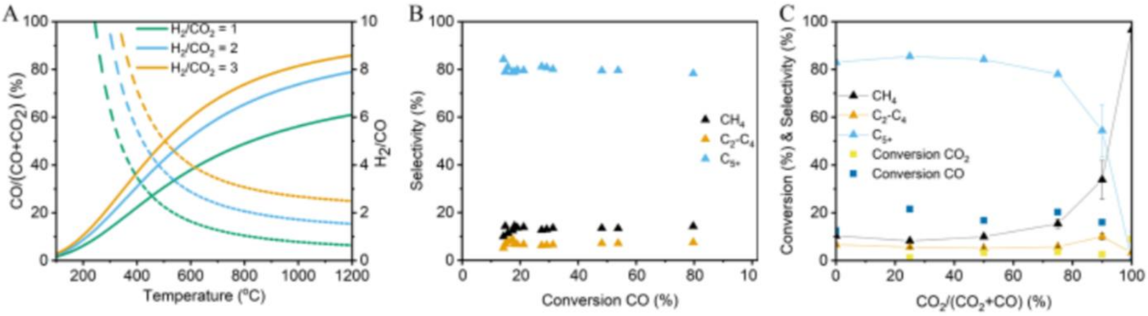

Figure 1. (A) Equilibrium compositions of the RWGS modelled with Aspen Plus, (B) Effect of CO conversion on selectivity for a 50% $CO_2/(CO+CO_2)$ feed H_2/CO_x 2/1 at 220 °C 21 bar in a PBR, (C) Effect of CO_2 content on selectivity H_2/CO_x 2/1 at 220 °C 21 bar in a PBR.

References

[1] World Economic Forum, & McKinsey. (2020). Clean Skies for Tomorrow Sustainable Aviation

Fuels as a Pathway to Net-Zero Aviation.
[2] Fan et al. Journal of Physical Chemistry Letters 2021 12 10486–10496.
[3] T. Riedel et al. Appl. Catal. A Gen. 1999, 186, 201–213.
[4] Y. Yao, et al. Industrial and Engineering Chemistry Research 2010, 49, 11061–11066.
[5] I. C. Have et al. Nat. Commun. 2022, 13

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Title: **[OP05]** Highly Active and Selective Borophene based catalysts for Reverse Water Gas Shift Reaction

Abstract: Since after its discovery, borophene, the two dimensional (2D) allotrope of boron, has remained as the latest sensation in flatland [1]. It is considered as the ‘new wonder material’ owing to its unique physical and chemical properties such as highly anisotropic electronic structure, mechanical compliance, ultrahigh thermal conductance, optical transparency and many more. Moreover, several theoretical calculations have shown that borophene can act as a superior catalyst for CO_2 reduction reactions, reduction of dinitrogen, hydrogen evolution reactions and many more [2]. However, there are very few experimental realizations yet, due to the lack of facile, low-cost and efficient synthetic methods. Present work describes a novel stepwise heating profile for the fabrication of borophene in very good yield [3].

Having developed a high yield route to borophene, we further focused on employing borophene as catalyst /support in heterogeneous catalysis, especially for the conversion of CO2 to value-added chemicals. We doped transition metals on borophene (M/Borophene; where M = Co, Fe, Ni, Cu and Ru) and investigated their catalytic activity towards Reverse Water Gas Shift rection (RWGS) (figure 1). RWGS is a promising process to produce syngas, a feedstock for a number of chemicals and fuels [4]. The results reveal that the catalysts are highly active, selective; and exhibit better performance compared to other 2D supported catalysts towards RWGS reaction [4]. To the best of our knowledge, no thermal reactions are reported so far using borophene based catalysts. Details of this work will be presented.

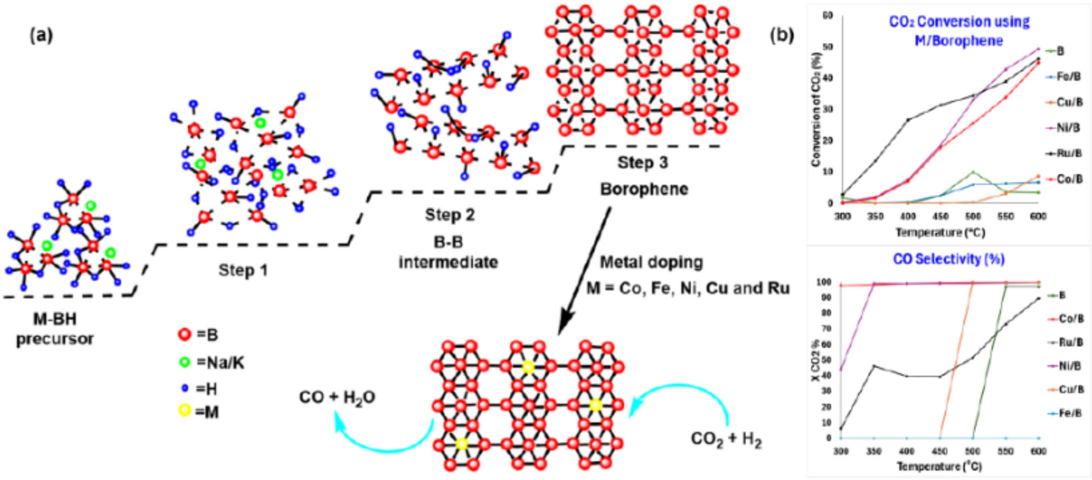

Figure 1: Schematic illustration of (a) synthesis of borophene and catalytic activity towards RWGS reaction; (b) results showing the % conversion and selectivity.

References

[1] P. Ranjan, J. M. Lee, P. Kumar, A. Vinu, Adv. Mater. 2020, 32, 2000531

[2] C. Hou, G. Tai, Y. Liu, Z. Wu, X. Liang, and X. Liu, Nano Research Energy, 2023, 2, e9120051.

[3] R. S. Anju, N. Raveendran Shiju, 2024, (Manuscript under preparation).

[4] a) M. Ronda-Lloret, L. Yang, M. Hammerton, V. S. Marakatti, M. Tromp, Z. Sofer, A. Sepúlveda-Escribano, E. V. Ramos-Fernandez, J. J. Delgado, G. Rothenberg, T. R. Reina and N. R. Shiju, , ACS Sustainable Chem. Eng., 2021, 9, 14, 4957-4966; b) T. Mathew, N. R. Shiju, ‘Survey of Heterogeneous Catalysts for the CO_2 Reduction to CO via Reverse Water-Gas Shift’ Chapter in the book ‘Engineering Solutions for CO2 Conversion’ ISBN: 978-3-527-34639-4, Wiley, March 2021.

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Title: **[OP06]** Supercritical CO_2 as effective wheat straw pretreatment for subsequent mild fractionation strategies

Abstract:

The efficient utilization of lignocellulosic biomass in biorefineries is pivotal for the transition to a carbon-neutral society, emphasizing the need for environmentally friendly fractionation techniques. While the extensive use of chemicals in biorefinery operations can yield favourable quantities of specific biomass components, adopting less chemically intense conditions is crucial for holistic methodologies that preserve the inherent potential of all biomass constituents. This study comprehensively investigates the use of supercritical carbon dioxide (sc-CO_2) as a green pretreatment to improve subsequent mild fractionation on wheat straw. Sc-CO_2 at 300 bars 100 °C and 70% moisture was found to have minimal impact on the chemical composition and the lignin structure, while there were significant morphological changes as heightened surface area and reduced density. Apart from increasing enzymatic saccharification efficiency, the treatment notably enhanced subsequent mild delignification through alkaline or inflow organosolv extractions. The combination of the pretreatments enhanced the lignin solubilization yields from 49 to 79% for alkaline and 74 to 91% for orgnaosolv, while retaining a high β-O-4 conservation of 49 and 59 linkages per 100 aromatic units. Additionally, the combined use of sc-CO_2 with mild dilute acid pretreatment improved xylose solubilization from 59 to 76% and enzymatic saccharification from 53 to 90%, albeit with increased lignin condensation. In summary, this study demonstrates the potential of sc-CO_2 pretreatment as a versatile tool for biomass valorization within the evolving bioeconomy, by combining enhanced extraction yields with minimal lignin structural impact. Our work thereby highlights the promise of the use of sc-CO_2 to contribute to the overall economic potential of biorefinery processes.

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Title: **[OP07]** Oxidative pretreatment as a way of upgrading cellulose-rich municipal waste streams

Abstract: Biomass will play an important role in the energy transition and is key for developing a sustainable future. More and more initiatives, not only in academic research but also in companies are putting efforts into using renewable carbon from biomass to produce valuable chemicals [1-2]. Certain municipal waste streams are a rich source of cellulose (tertiary cellulose), for example, toilet paper-rich side streams from waste water purification plants. This carbon feedstock has a great potential to be a valuable feedstock with minimal carbon footprint and the reintroduction of waste to the economy [3-4]. For that, pretreatments are necessary to remove contaminants before further conversion by, for example, thermochemical or biotechnological approaches [5]. In our investigation, we performed oxidative pretreatments using tertiary cellulose (Recell®) provided by the Recell Group B.V. These involved the use of ozone, hydrogen peroxide, and sodium hypochlorite and the results were compared with an alkaline pretreatment. Detailed characterization of the products was performed using a wide range of techniques to obtain process-product property relations. In addition, the use of the pretreated products for glucose synthesis using an enzymatic treatment was also assessed to select the most promising pretreatment technique and these results will also be presented.

References

[1] “Cellulose, the new direction for our basic chemistry”, Recell®, accessed 26 June 2024, https://recell.eu/nl/markten/#recell-chem.

[2] “FDCA and plantMEGTM together make a 100% plant-based plastic PEF”, Avantium, accessed 26 June 2024, https://avantium.com/business-units/renewable-chemistries/.

[3] “Count to three and win the most!”, Recell®, accessed 26 June 2024, https://recell.eu/the-how-and-why-of-tertiary-cellulose/.

[4] R. Liu, Y. Li, M. Zhang, X. Hao, and J. Liu, “Review on the fate and recovery of cellulose in wastewater treatment,” Resour. Conserv. Recycl., vol. 184, no. 106354, p. 106354, 2022.

[5] Z. Zhou, D. Ouyang, D. Liu, and X. Zhao, “Oxidative pretreatment of lignocellulosic biomass for enzymatic hydrolysis: Progress and challenges,” Bioresour. Technol., vol. 367, no. 128208, p. 128208, 2023.

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Title: **[OP08]** Complete liquefaction of enzymatic hydrolysis lignin via non-catalytic solvolysis

Abstract: Lignocellulose, containing cellulose, hemicellulose and lignin, is the most abundant biomass material on the Earth for the production of biofuels. The second-generation (2G) biorefineries have successfully produced bio-ethanol as a gasoline blend using cellulose and hemicellulose but leaving enzymatic solvolysis lignin (EHL) as a solid waste. EHL, as a large-scale industrial waste, exhibits promising potential as a feedstock to produce biofuels for the development of sustainability and profitability of the 2G biorefineries. However, EHL has complex and heterogeneous nature and shows low solubility in common solvents resulting in a persistent barrier to its effective utilization. In this work, the non-catalytic EHL solvolysis method was examined in methanol, ethanol, isopropanol, and their mixtures with H_2O. Notably, the complete EHL liquefaction was achieved in an isopropanol-H_2O mixture without char formation. The liquefaction degrees of EHL in different solvents are displayed in Figure 1 (a). The monomer products of EHL non-catalytic solvolysis in different solvents are shown in Figure 1 (b) and (c). The major monomers are para-ethyl and vinyl-substituted phenol and guaiacol. The interactions between EHL and the solvents and the specific roles of isopropanol and H2O in EHL liquefaction were investigated using operando HSQC-NMR spectroscopy and molecular dynamics simulations. In the EHL solvolysis process, H_2O disrupts the hydrogen bonds in EHL and isopropanol break π-π stacking interactions between the aromatic rings in EHL. H_2O also enhances EHL depolymerization, while isopropanol, as a hydrogen donor solvent, provides hydrogen that stabilizes active intermediates.

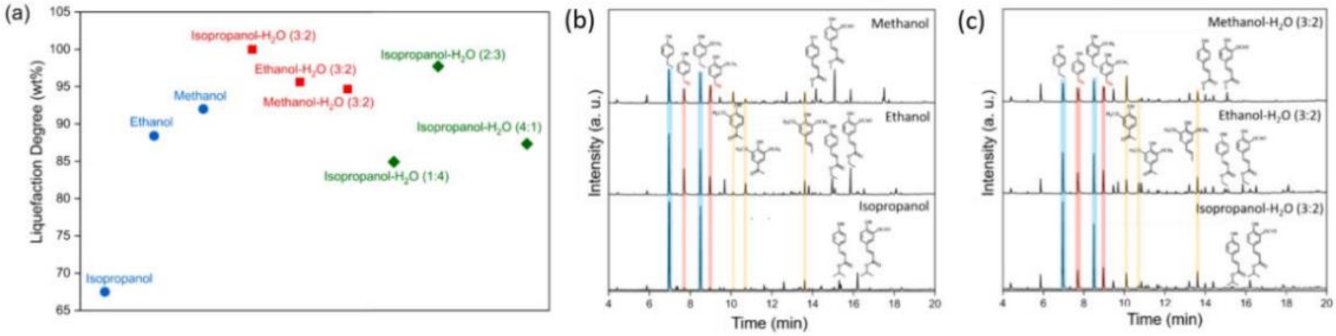

Figure 1. (a) EHL liquefaction degree in different solvents. (b) Monomer products of EHL solvolysis in pure alcohol solvents. (c) Monomer products of EHL solvolysis in alcohol-water mixture solvents.

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Title: **[OP09]** A Sustainable Process Design For The Production of Nitrile Butadiene Rubber for Medical Glove Usage

Abstract: The trade-off between the environmental impact of single-use medical gloves and the inherently unique properties of the material that they are made of (nitrile butadiene rubber, NBR) presents itself to be one of the greatest 21st century challenges. In The Netherlands, 7%
of the national footprint is associated with this sector [1]. From this hotspot, nitrile gloves account for one of the highest carbon footprints (9.3 kg CO_2-eq/kg nitrile) and water usage (60 kg water/kg nitrile) [2] [3]. By aligning into the United Nations' Sustainable Development Goals [4], and addressing the emission hotspot of the medical gloves, a novel process design is proposed, which greatly reduces the environmental impact.

This innovative process design addresses the production of the base monomers (acrylonitrile and butadiene), their polymerization, and the glove manufacturing. Firstly, two renewable sources are chosen as raw materials: The production process of acrylonitrile involves the usage of glycerol, obtained as a byproduct in the production of bioethanol. The production of butadiene entails a biological process with glucose obtained from sugar beets.

Secondly, apart from choosing more sustainable raw materials, some subprocesses were integrated, with the goal of improving and optimizing the base design. These propositions include combining infrared (IR) and vacuum drying for the manufacturing stage of the gloves to replace the conventional heat-drying, recirculation of a wastewater stream into the fermentation process and heat recovery and acrolein recycling for the acrylonitrile process. In addition, two innovative equipment designs are suggested: a vessel that combines decantation and filtration as a glycerol purification unit and an absorption falling film reaction in-situ vessel for the simultaneous production of acrylonitrile and separation of acrylonitrile from ammonia and acrolein.

The final Cradle-to-Grave concept aims to capture 20 percent of the EU market share of nitrile gloves. The plant capacity was equivalent to 1980 tonnes/year of resin (NBR) production, which was the reference value for the process design calculations. According to this, the concept was evaluated in terms of Sustainability and its contribution to UN's SDGs #6 (for sustainable water management) and #9 (for sustainable production patterns) [4]. An environmental impact assessment by LCA was performed, which showed a reduction of CO_2-eq emissions of 25%, and a 29% reduction in water consumption for the proposed design compared to the conventional method. These results not only address the SDG #6, they specifically target 6.4 (increasing the water-use efficiency) but also cover SDG #9, specifically target 9.4 (minimizing the environmental impact by promoting industrial circularity and project robustness).

Finally, an economic assessment was conducted, in which the Zero Order Economic Potential (EP0) of the designed linear chain (14. 7M€/y) was compared to a supply chain industrial

symbiosis where a 15% increase was noticed (EP0 = 17 M€/y), suggesting that promoting circularity would be beneficial both from an environmental and a financial standpoint.

References

[1] Gupta Strategies, "Transition to a sustainable healthcare sector," Gupta Strategies, [Online].Available:https://gupta-strategists.nl/en/research/een-stuur-voor-de-transitie-naar-duurzame-gezondheidszorg.
[2] N. Hunfeld, J. C. Diehl, M. Timmermann, P. v. Exter, J. Bouwens, S. Browne-Wilkinson, N. d. Planque and D. Gommers, "Circular material flow in the intensive care unit—environmental effects and identification of hotspots," Intensive Care Medicine, vol. 49, pp. 65-74, 2022.
[3] N. Hunfeld, J. C. Diehl, S. V. D. Zee, D. Gommers and E. M. v. Raaij, "The Green Intensive Care: From Environmental Hotspot to Action," ICU Management & Practice, vol. 23, no. 3, pp.106-109, 2023.
[4] United Nations, "The 17 goals," United Nations, [Online]. Available: https://sdgs.un.org/goals.

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Title: **[OP10]** Generative artificial intelligence (AI) in chemical process engineering

Abstract:

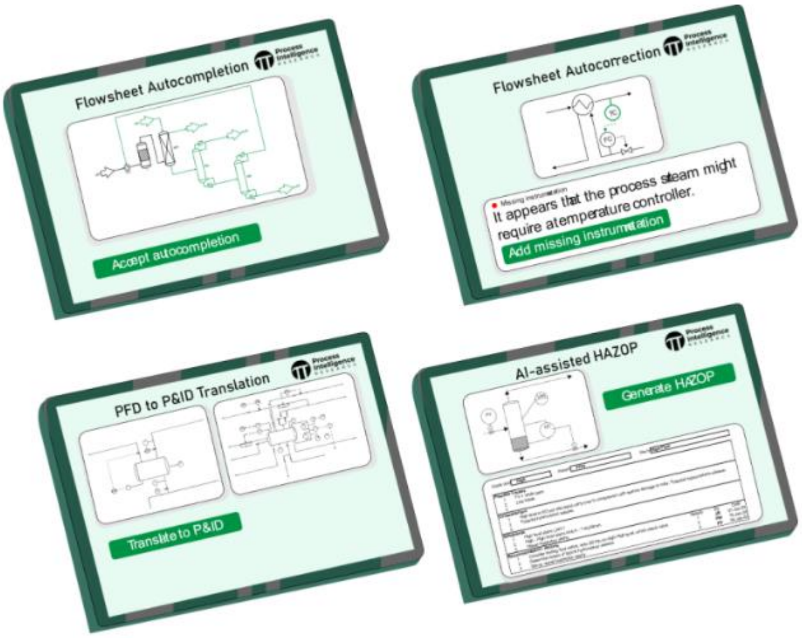

Figure: Illustration of generative AI applications in chemical process engineering.

I envision that generative artificial intelligence (AI) will have a considerable impact on chemical process engineering. Generative AI has gained immense traction across diverse sectors, exemplified by ChatGPT's language generation and GitHub Copilot's code generation. Generative AI also holds immense potential to reshape chemical process engineering by offering advanced data handling, modeling, and decision-support capabilities, ultimately driving innovation and efficiency in the industry. However, there are only limited applications in chemical engineering so far. I propose applications for generative AI in process engineering including autocompletion of flowsheets, autocorrection of engineering documents, P&ID generation, and AI-assisted HAZOPs. In my view, we need to conduct research and development in three main areas to ultimately develop useful generative AI tools in our domain: (1) data, (2) information representation, (3) model architectures including mechanistic information.

References

[1] Schweidtmann, A. M. (2024). Generative artificial intelligence in chemical engineering. Nature Chemical Engineering, 1(3), 193-193.

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Title: **[OP11]** Understanding the Selectivity of Bicarbonate Electrolysis

Abstract: Bicarbonate electrolysis is a promising method to integrate carbon capture directly with electrochemical conversion. By using an alkaline capture solution, CO_2 can be capture in the form of bicarbonate and directly used as electrolyte for the electrolyser to generate CO. Most research has focused on improving the faradaic efficiencies of the system, however, the selectivity over time has not been addressed properly[1, 2]. Therefore, in this work we aim at understanding the CO selectivity as function of time in a bicarbonate electrolyser as well as investigating the role of the electrolyte pH.

The bicarbonate electrolyser was optimized by introducing a spacing between the electrode and the membrane. A better local pH gradient was obtained, improving both the CO_2 liberation at the membrane and the CO_2 reduction conditions at the electrode. A good bicarbonate electrolyser performance was achieved, however, a large decrease in selectivity over time was observed. It was hypothesized that the change in bulk pH plays a major role the stability of the bicarbonate electrolyser. Therefore, to understand the role of the electrolyte pH, several experiments with single-pass electrolytes at various bulk pH conditions were studied. We found that the bulk pH strongly effects the overall selectivity, where a more alkaline electrolyte reduces the selectivity toward CO. However, the bulk pH does not control the stability of the system. Instead, it was found that the deposition of trace metal ion impurities which are present in the high concentration electrolyte salt are the main cause for the decrease in selectivity [3]. By complexing these trace metal ions with ethylenediaminetetraacetic acid (EDTA), the metal deposition was avoided and a stable CO selectivity was obtained.

Based on the current findings, the importance of improving the performance of the bicarbonate electrolyser at higher pH conditions is stressed. For the effective integration of a bicarbonate electrolyser with an alkaline capture step, the connecting liquid streams must be compatible with the operating conditions of both separate systems. Therefore, a better performance of the bicarbonate electrolyser at higher pH conditions is crucial to make the process integration possible. This work is a first step at understanding the operation of the bicarbonate electrolyser at different pH inlet conditions.

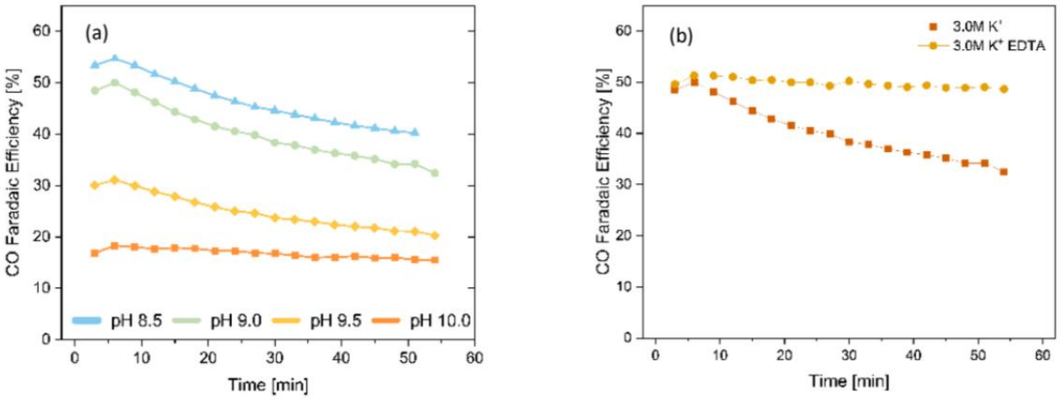

Figure 1 Bicarbonate electrolysis using a Ag spray-coated cathode and 3M $KHCO_3$ catholyte at a constant applied current of 100 mA/cm^2, and a fixed spacing of 135 µm between the membrane and the cathode. Faradaic efficiencies towards CO for (a) different constant pH inlet conditions, (b) constant electrolyte at pH 9 with and without the addition of 0.02 M EDTA.

References

[1] E. W. Lees, M. Goldman, A. G. Fink, D. J. Dvorak, D. A. Salvatore, Z. Zhang, N. W. X. Loo, C. P. Berlinguette, ACS Energy Letters 2020, 5, 2165-2173.

[2] T. Li, E. W. Lees, M. Goldman, D. A. Salvatore, D. M. Weekes, C. P. Berlinguette, Joule 2019, 3, 1487-1497.

[3] A. Wuttig, Y. Surendranath, ACS Catalysis 2015, 5, 4479-4484.

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Title: **[OP12]** Modification of stainless-steel as bifunctional electrocatalysts towards high active and stable anion-exchange membrane water electrolysis

Abstract: The increasing awareness of the need to mitigate the impact of global warming and climate change is spurring the adoption of clean and renewable energy sources [1]. Among the promising technologies for harnessing renewable energies (such as solar, wind, and hydro) to foster a sustainable future, water electrolysis stands out. This process can produce hydrogen gas, an efficient energy carrier and an alternative to fossil fuels for power generation [2]. Currently, three types of low-temperature water electrolyzers have been developed: conventional alkaline water electrolyzers (AWE), proton exchange membrane (PEM) water electrolyzers, and anion exchange membrane (AEM) water electrolyzers. The AEM water electrolyzer can represent a significant advancement as it combines the benefits of both AWE and PEM electrolyzers. It enables the use of non-noble-metal electrocatalysts, similar to AWE, and incorporates a high-performance membrane separator, akin to PEM electrolyzers [3]. Despite these advantages, the AEM electrolyzer is still in the early stages of development, and there is ample room for reducing the total device capital costs, as well as improving its efficiency, particularly when employing non-noble-metal catalysts [4]. Low-cost stainless steel is becoming a promising electrode material for green hydrogen production through alkaline water electrolysis [5]. Herein, the electrocatalytic performance of 304-type stainless steel meshes in AEM cells was enhanced through a simple two-step activation process, i.e., chemical etching followed by electrochemical activation. The modified electrodes exhibited comparable hydrogen and oxygen evolution reaction properties to noble metal-based electrodes, requiring a >300 mV lower cell voltage than the unmodified stainless steel-based cells to sustain a constant current of 5.0 A (1.0 A cm^{-2}). Electrochemical impedance spectroscopy studies showed a significant decrease in interfacial contact, charge transfer, and mass transport resistances. Characterization by x-ray photoelectron spectroscopy and transmission electron microscopy of the modified stainless-steel surface revealed the presence of nanocrystalline Fe-NiCr LDH and $Ni(OH)_2/Fe(OH)_2$ species when used in hydrogen and oxygen evolution side, respectively, which may explain the significantly higher. Moreover, the long-term durability of the modified electrodes was assessed in a continuous flow electrolyzer where exceptional stability was observed at a constant current of 5.0 A (1.0 A cm^{-2}) for 250 h. Due to its simplicity and cost-effectiveness, the proposed modification of stainless-steel electrodes has the potential for upscaling and deployment in the next- generation, low-cost AEM systems.

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References
[1] Jiang, W., et al., Advanced Functional Materials (2022) 32 (38), 2203520
[2] Jiang, T., et al., Journal of Materials Chemistry A (2022) 10 (44), 23863

[3] Jang, M. J., et al., ACS Energy Letters (2022) 7 (8), 2576
[4] Wang, F.-L., et al., Applied Catalysis B: Environmental (2023) 330, 122633
[5] Chen, B., et al., ACS Energy Letters (2023) 8 (6), 2661

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Title: **[OP13]** A computational study on the impact of electrolyzer geometry on the Faradaic efficiency of alkaline water electrolyzers

Abstract: Green hydrogen production through water electrolysis has the potential to lead the decarbonization of energies for it is a zero emission fuel produced from renewable energy sources (RES). Upon this matter, alkaline water electrolysis (AWE) stands as an attractive technology since it relies on relatively unexpensive materials.

Yet, the fluctuating nature of RES poses a significant challenge on its integration to AWE systems as this forces the electrolyzer to temporarily operate at partial nominal loads, which spawns several engineering problems regarding process safety, energy efficiency and corrosion of materials.

Particularly, shunt currents become a serious issue, as they increase at partial loads and are responsible for faradaic efficiency losses and corrosion on manifold pipes (Sakas, 2024). Therefore, minimization of these parasitic pathways can help improve on the electrolyzer integrity and efficiency. An schematic of the shunt currents propagation is presented in Fig 1.

This work provides a computational approach to study the shunt current behavior with different geometric configurations of the stack ensemble (manifold and inlet/outlet ports). An equivalent circuit model has been utilized alongside a current-voltage model to predict the expected shunt currents.

Thermodynamic aspects of the electrolyte solution as well as the effect of gas accumulation in the outlet pipes were included for a more realistic description of the system. The results showed that a careful design of the electrolyzer ensemble could significantly improve the Faradaic efficiency.

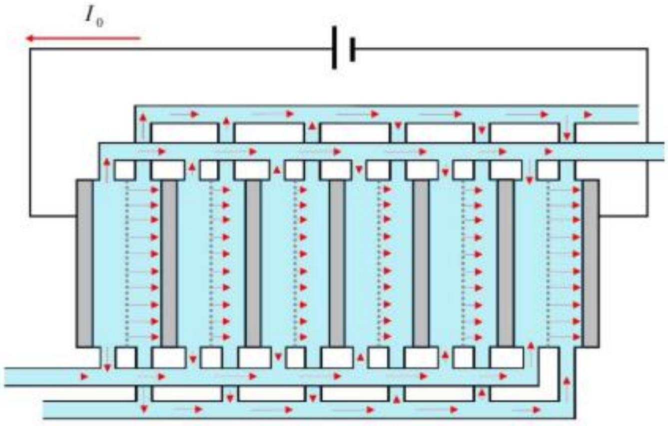

Figure 1. Illustration of the current transport on a bipolar-plate electrolyzer.

References

[1] Sakas, G., Ibáñez-Rioja, A., Pöyhönen, S., Kosonen, A., Ruuskanen, V., Kauranen, P., & Ahola, J. (2024). Influence of shunt currents in industrial-scale alkaline water electrolyzer plants. Renewable Energy, 225, 120266. https: //doi.org/https:// doi.org/ 10.1016/ j.renene. 2024.120266

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Title: **[OP14]** Improved colloid stability of polymer microspheres by low temperature deposited nanofilms of SiO_2 in fluidized beds

Abstract: Fine particles dispersed in a liquid medium have extensive applications in various fields, including food, drug delivery, and paints[1]. Ideally, water would be the medium in which particles are dispersed; however, not all solids are naturally compatible with polar media. In our study, we utilized the atomic layer deposition (ALD) coating technique to deposit nanofilms of SiO_2 on polymer microspheres with the aim of improving their colloid stability in water[2]. The ALD process, where sequential pulses of chemicals react in a self-limiting manner with the surface groups of the substrate's surface, allows for molecular precision when depositing film. By applying these extremely-thin nanofilms, surface properties can be modified while bulk properties remain unaffected. Given the granular nature of our substrate, we performed this coating in a fluidized bed reactor. After deposition, we used various techniques to characterize the newly formed surfaces and their affinity with water. Surface characterization by Fourier transform infrared spectrometry (FTIR) and X-ray photoelectron spectrometry (XPS), revealed the presence of a large number of deposited hydrophilic Si-OH groups within the first cycles. Utilizing environmental scanning electron microscopy (ESEM) allowed visualization of pristine and coated particles in the presence of water, revealing a stark contrast in affinity after deposition. Furthermore, focused beam reflectance measurements (FBRM) showed a significant decrease in agglomerate size of coated particles in water compared to pristine ones, indicating a higher colloid stability. Finally, water contact angle (WCA), and droplet absorption time of the powder were measured, which also showed an improved water-substrate affinity.

We observed an increase in the amount of Si-OH present on the particle surface with an increasing number of deposition cycles, however no significant improvement in water affinity was found after the first coating cycles. Since it was found that full surface coverage was achieved within 2 coating cycles, it was concluded that surface overage is the primary factor in improving colloid stability by means of SiO_2 nanofilm deposition.

References
[1] T.F. Tadros, https://doi.org/10.1002/9783527631179.ch1
[2] R. Kamphorst et al., https://doi.org/10.1016/j.surfin.2024.103852

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Title: **[OP15]** Preparation and Selected Applications of Polymer Thin Films Synthesized by Initiated Chemical Vapor Deposition (iCVD)

Abstract: Initiated chemical vapor deposition (iCVD), an evolution of traditional CVD methods, has emerged as a pivotal technology for polymer synthesis. Offering solvent-free, room-temperature deposition, iCVD enables the generation of conformal, precisely tunable surfaces on diverse substrates without causing damage. Furthermore, a large variety of unsaturated species are available for use as monomers through free radical polymerization, and iCVD makes it possible to preserve the functional integrity of monomers.

In this study, we utilized iCVD to fabricate poly (allyl methacrylate) (PAMA) thin films and explored their potential for creating compositional gradients and enhancing interfacial adhesion. Polymer gradient materials exhibit a gradual change in composition along one or more directions, resulting in a gradual change in material properties. iCVD is an excellent approach for creating gradient structures on the nanoscale by precisely controlling deposition parameters, allowing for the acquisition of entirely new physical and chemical properties.

We fabricated the gradient polymer thin films by accurately controlling the flow rates of two monomers, allyl methacrylate (AMA) and N, N-Dimethylacrylamide (DMAA), throughout the iCVD process. The quality and homogeneity of the films were studied through SEM and profilometry. FTIR, XPS, EDS, and water contact angle measurements confirmed the presence of the compositional gradient and the retention of allyl functional groups in the polymer. Mechanical properties were assessed using AFM. The feasibility of spatial control on crosslinking was demonstrated through radiation exposure using a photomask, indicating the potential for fabrication based on lithography techniques.

The promotion of interfacial adhesion is essential for attaching two different materials. The most popular means of surface modification are solvent-based and laser methods. However, these methods are prone to damaging chemically and thermally susceptible substrates, which greatly limits their practical application. In terms of substrate-independent surface coatings and nondestructive methods, iCVD serves as an attractive means to design rational functional surfaces [1]. PAMA thin films act as an adhesion promoting layer, which strongly adheres to the substrate and has well-preserved allyl functional groups on the surface due to the unique advantages of iCVD. The UV-curable thiol-ene adhesives we prepared can be covalently linked with PAMA during the curing process via click chemistry. The solvent-free and mild adhesion network significantly improves the adhesion strength, which opens a novel avenue for eco-friendly adhesives on different substrates.

References

[1] S. J. Yu et al., Advanced Engineering Materials 2018, 20.

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Title: **[OP16]** Diels Alder and domino reactions for self-healing materials

Abstract: The success of self-healing telechelic or polymeric networks depends on the polymeric architecture, including the polymeric backbone, the functionality of branching units and the cross-link density. These are among the key factors determining the final mechanical properties of the material, as well as the self-healing performance. In this work, a method is proposed to balance the self-healing performance and mechanical properties in a simple supramolecular furan-maleimide system. By applying a post-curing step, the functionality of the branching unit is increased by using the double Diels-Alder reaction. As opposed to the method of introducing an extra cross-linker, bottlenecks such as heterogeneity in the system can be avoided as DDA introduces new branching points homogeneously over the network. Here we demonstrate how a post-curing step below the gel transition temperature of such materials affects the glass transition temperature, network mobility, tensile properties and self-healing efficiency. The post-curing step is followed in three situations: i) in presence of excess maleimide, ii) in presence of a 1:1 furan-maleimide ratio and iii) having an excess of furan. Using infrared spectroscopy, rheometry, and broadband dielectric spectroscopy the double Diels-Alder reaction is investigated during the post-curing step in this comprehensive study. We propose double Diels-Alder for designing new telechelic Diels-Alder networks with any functionality of the branching unit, while the chemical structure of the backbone remains identical.

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Title: **[OP17]** Techno-economic and environmental impacts of replacing fossil-based processes in the propylene subcluster in the Port of Rotterdam

Abstract: Alternative carbon sources (ACS) such as CO_2, biomass, and waste, are promising options to defossilise existing chemical processes. However, ACS processes need additional or different material and energy streams than existing fossil-based processes, within and outside their value chains, leading to new interconnections and cascading impacts on the overall techno-economic and environmental (TEE) performance of the existing subclusters. Thus, it is crucial to examine how the overall performance of the subcluster is affected when defossilising one or several value chains. This research examines the TEE impacts associated with defossilising three value chains of downstream derivatives: methyl tert-butyl ether (MTBE), propylene glycol (PG), and polyol, which are part of the propylene subcluster in the Port of Rotterdam (the Netherlands).

The three fossil-based value chains were modelled to match the real capacities, conditions and interconnections in the Port using Aspen Plus v12. To defossilise the downstream derivatives in these chains, three ACS processes were modelled: bio-MTBE, bio-PG, and CO_2-based polyol. The performances of the ACS-based and fossil-based processes were compared using the following indicators: mass and energy intensity, water consumption, land requirements, capital and operational costs, and CO_2 emissions. To evaluate potential cascading impacts at the subcluster level, a scenario tree was developed outlining strategies for (i) the deployment of ACS processes (e.g., one at a time or all together) and (ii) utilizing unused intermediate chemicals inside/outside the subcluster (e.g., due to changes in production capacities when switching from fossil to ACS processes). Then, the cascading impacts were examined by (i) identifying changes in the interconnections within and beyond the current value chains, and (ii) analysing their effects on the subcluster's TEE performance. The results highlight significant changes in the material and energy profiles. We found that current energy flows would be insufficient to meet the needs of the ACS-based processes, therefore resulting in higher utility consumption, such as in heating and cooling needs, nitrogen and hydrogen demands. Using ACS processes for the production of polyol, PG and MTBE reduces the need for intermediate chemicals produced currently within the subcluster, thereby impacting upstream and downstream flows (e.g., capacities of the processes). The results show that replacing fossil-based processes with ACS processes can significantly affect the performance of the propylene subcluster and highlight the need to analyse ACS impacts beyond the boundaries of single processes.

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Title: **[OP18]** Exploring the synergistic integration of CO_2 electrolysis and CCS supply chains for sustainable syngas production

Abstract: The production of syngas (a chemical building block of carbon monoxide and hydrogen) via high-temperature (HT) co-electrolysis (CO_2E) of steam and CO_2 shows great potential to reduce the reliance on fossil fuels within the chemical industry (Gabrielli et al., 2023). CO_2E could operate independently of fossil fuels by using renewable energy and CO_2 from biogenic sources or the atmosphere. CO_2E has yet to be implemented on an industrial scale as both the technology (TRL 5-6) and its associated supply chain are currently under development.

CO_2E and carbon capture and storage (CCS) share the initial supply chain stages, where CO_2 is captured at the emission source, compressed, and transported to a conversion or storage site. However, CCS is at TRL 9 (Kearns et al., 2021). Several industrial-scale European projects are expected to be operational before 2030 (Northern Lights, 2023; Porthos, 2024). Given the common elements of both supply chains, integrating them could lead to significant synergistic benefits from developing a shared infrastructure (Dahlgren et al., 2013), for instance, in CO_2 pipeline transport. An additional network integration advantage is that the CO_2 supply can be guaranteed to align with renewable energy availability. When the electrolyzer is not operational, CO_2 can be stored permanently instead of used. However, scaling up CO_2 utilization and storage might encounter challenges due to competition for the same CO_2 sources. Moreover, the scale at which CCS is employed is envisioned as an order of magnitude larger than that of utilization (IPCC, 2022). This could shape the CO_2 supply chain in a way that is not optimal for utilization, for example, with CO_2E being an addition to CCS. To understand the benefits and challenges of developing synergistic CO_2 utilization and storage supply chains, a facility location and configuration model has been developed using GAMS. This model analyses various syngas production and CO_2 storage targets to identify optimal supply chain configurations. These supply chain configurations are analysed based on the CO_2 sources used, connections between sources and end-use, and the size of the electrolyzer and permanent storage. The resulting mixed integer linear programming (MILP) model aims at optimizing the supply chain based on economic and environmental objectives, i.e., the annualized cost of the system and global warming potential (GWP). The goal is understanding the trade-offs between CO_2 conversion (specifically CO_2E) and storage. This work contributes to determining if there are conditions where both can achieve mutual benefits while also balancing cost-efficiency and environmental sustainability.

References

[1] Dahlgren, E., Göçmen, C., Lackner, K., & Van Ryzin, G. (2013). Small modular infrastructure. Engineering Economist, 58(4), 231–264. https://doi.org/10.1080/0013791X.2013.825038

[2] Gabrielli, P., Rosa, L., Gazzani, M., Meys, R., Bardow, A., Mazzotti, M., & Sansavini, G. (2023). Net-zero emissions chemical industry in a world of limited resources. One Earth, 6(6), 682–704. https://doi.org/10.1016/j.oneear.2023.05.006

[3] IPCC. (2022). Climate change 2022: Impacts, adaptation and vulnerability. IPCC Sixth Assessment Report.

[4] Kearns, D., Liu, H., & Consoli, C. (2021). Technology Readiness and Costs of CCS. Global CCS Insitute, March, 50. https://www.globalccsinstitute.com/wp-content/uploads/2021/03/Technology-Readiness-and-Costs-for-CCS-2021-1.pdf

[5] Northern Lights. (2023). Annual Report 2023.

[6] Porthos. (2024). Project. https://www.porthosco2.nl/project/

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Title: **[OP19]** Numerical and Experimental Study of the Axis-Switching Phenomena in Rectangular Jets

Abstract: Rectangular jets exhibit axis-switching behavior, which leads to enhanced flow entrainment compared to round jets. This axis-switching behavior makes rectangular jets promising in industrial applications where efficient mixing is required as they can serve as effective passive flow controllers. However, despite their advantages, rectangular jets have not been studied as extensively as round jets [1-3]. To be able to use rectangular jets in practical applications, a more comprehensive understanding of the underlying phenomena influencing the axis-switching behavior is required.

In this study, we perform Direct Numerical Simulations (DNS) of rectangular jets at various injection velocities. To accurately track the liquid-gas interface, we employ the Local Front Reconstruction Method (LFRM) [4]. This simulation technique allows for a detailed description of the gas-liquid interface at relatively low computational cost.

Our simulations are validated against experimental data obtained within similar ranges of Weber and Reynolds numbers. Our simulation results show a good correspondence with the experimental data, which demonstrates that LFRM is capable of accurately capturing the physical phenomena involved in the break-up of a rectangular jet, such as the jet oscillations, break-up lengths, and droplet sizes.

To study the effect of the velocity profile at the nozzle outlet on jet deformations, we investigate the impact of a fully developed and uniform velocity profile in the jet dynamics. We observe that a fully developed velocity profile at the nozzle outlet leads to enhanced jet stability, which in turn results in larger break-up lengths. In contrast, jets with a uniform velocity profile exhibit shorter break-up lengths and, therefore, manifest less stability. Axis- switching and flow entrainment are observed for both velocity profiles, where the flat velocity profile enhances flow entrainment. Additionally, the simulation results reveal time-coherent azimuthal and stream-wise vortices, which promote flow entrainment.

This research provides a detailed analysis of the axis-switching behavior and associated dynamics of rectangular jets using Direct Numerical Simulations. The break-up length, droplet sizes, and oscillating wavelength from the simulations show good agreement with the experimental data, which demonstrates that LFRM is a suitable technique for simulating rectangular jets. The results obtained in this work showed that the velocity profile at the nozzle plays an important role in the jet stability and break-up length. Future research should be performed to explore the parameters influencing rectangular jet behavior.

References

[1] F. Wang and T. Fang. Liquid jet breakup for non-circular orifices under low pressures. International Journal of Multiphase Flow, 72: 248–262, 2015.

[2] Jaberi and M. Tadjfar. Wavelength and frequency of axis-switching phenomenon formed over rectangular and elliptical liquid jets. International Journal of Multiphase Flow, 119:144–154, 2019.

[3] M. Tadjfar and A. Jaberi. Effects of aspect ratio on the flow development of rectangular liquid jets issued into stagnant air. International Journal of Multiphase Flow, 115:144–157, 2019.

[4] S. Shin, S. I. Abdel-Khalik, V. Daru, and D. Juric. The Local Front Reconstruction Method for direct simulation of two- and three- dimensional multiphase flows. Journal of Computational Physics, 2011.

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Title: **[OP20]** Systematic methodology via a decision matrix for the quick selection of energy-efficient intensified distillation technologies

Abstract: Distillation is the most widely used separation technology in chemical industries. However, because of its relatively low thermodynamic efficiency, distillation accounts for around half of the operational costs of chemical plants [1]. To reduce the operational costs as well as the capital costs, advanced distillation techniques based on process intensification (PI) are considered highly competitive in terms of enhancing the energy efficiency and economic performance by integrating unit operations or functions. Such technologies include heat pump assisted distillation, heat integrated distillation, membrane assisted distillation, high gravity distillation, cyclic distillation, thermally coupled distillation systems, dividing wall column, extractive distillation and azeotropic distillation. However, matching suitable intensified distillation techniques with given separation tasks based on a wide range of application cases remains a challenge. Commenge and Falk developed a framework for selecting the right intensified techniques for reaction equipment [2], but no general methodology that allows the selection of the most promising PI technologies for different separation tasks, prior to process synthesis, design or optimization.

This study is the first to generate a conceptual multi-step selection and decision approach by first going through several high level questions with corresponding suggested solutions for a separation task in order to identify special components (e.g., non-condensable or thermosensitive, or with the risks of solidification). Then the process bottlenecks and intensification targets via a list of evaluation criteria (boiling point difference, distillation sequence efficiency, etc.) are identified. Each of the technologies are entered into a pre-filled matrix, and are scored based on the relevance to the evaluation criteria. Finally, the most promising intensified technologies are recommended based on their scores, and potential solutions are compared against the task specifications. The PI matrix proposed in this work aims to yield a short list of appropriate solutions to be designed and economically assessed, proposing a screening framework for fluid separations in order to make a rapid selection at an early stage. Several binary, ternary, and multicomponent zeotropic and azeotropic mixture separations are carried out as case studies to illustrate the application of the proposed methodology. The list of the promising intensification technologies gained from the developed approach are confirmed by the PI techniques reported in the literature, yet without carrying out any simulations or designs, showing rapid and reliable selections of the most promising distillation techniques. This methodology contributes to integrating a wide range of evaluation criteria, and providing a basis for the selection of technologies at an early design stage. This screening can also act as a decision making tool in the pre-selection step for the synthesis or optimization methodologies to help dramatically reduce the search space.

References

[1] Kiss, A.A., Landaeta, S.J.F. and Ferreira, C.A.I., 2012. Towards energy efficient distillation technologies–Making the right choice. Energy, 47(1), pp.531-542.

[2] Commenge, J.M. and Falk, L., 2014. Methodological framework for choice of intensified equipment and development of innovative technologies. Chemical Engineering and Processing: Process Intensification, 84, pp.109-127.

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Title: **[OP21]** Modelling and Analysis of Electrolysers Integrated with Downstream Separation Systems via Heat Pumps

Abstract: The electrification of chemical processes represents an attractive pathway to enhance efficiency and leverage waste heat, while at the same time, possibly, introducing flexible operational frameworks. Electrolysers could play a central role in this transition, as they would allow for hydrogen production from renewable sources but also hold potential for converting CO_2 into valuable products. A significant challenge, however, lies in effectively utilizing the low-temperature heat (60-80 °C) dissipated by the electrolysers, corresponding to around 30-40% of the power input to the stacks (Dal Mas, 2024, Front. Energy Res.). Our project addresses this challenge by modeling a system that integrates electrolysers with downstream separation processes, utilizing heat pumps to upgrade the waste heat from the electrolysers and drive the separation process. The investigation is based on the steady-state model of a system comprising several electrolyser stacks, a balance of plant, and a distillation unit required to separate the desired product and recycle unreacted water and the electrolyte. The case study considered is the production of formic acid through direct CO_2 electrolysis, as this process could be more readily implemented at relevant industrial scales (Dal Mas, 2024, Comput. Aided Chem. Eng.). Ensuring that the energy requirements of the downstream processes were met by the upgraded waste heat from the electrolysers was a crucial aspect of this model, optimizing overall system efficiency. Through our research, we developed a steady-state simulation model integrating electrolysis and downstream separation systems with heat pumps. The simulations and analyses were conducted using Aspen Plus. Our project offered valuable insights into the efficient integration of electrolysers and downstream processes, emphasizing the role of heat pumps in enhancing system performance and energy utilization (based on 50 MW power input to the electrolyser, a COP of 4 was obtained through the application of compression/resorption heat pumps). In addition to steady-state analysis, the aim of the work is also to conduct dynamic simulations to understand the system's response to various disturbances, including partial shutdowns and subsequent startups of the electrolysers. This dynamic study will evaluate how such fluctuations impact separation performance and energy demand, with a particular focus on the performance of the heat pumps.

References

[1] Dal Mas, Riccardo, et al., 2024. “Challenges and Opportunities for CO_2 Electroreduction from a Process Systems Engineering Perspective.” Frontiers in Energy Research 12 (March):1340622.

[2] Dal Mas, Riccardo, et al., 2024. “Evaluation of energy requirements for chemicals and fuels manufactured via electrochemical reduction of carbon dioxide.” Computer Aided Chemical Engineering 53.

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Title: **[OP22]** Performance assessment for the Twente-DAC pilot using sorbent circulation

Abstract: Direct Air Capture (DAC) is essential for achieving net-zero carbon emissions by addressing rising CO_2 levels and contributing to climate change mitigation. Using harvested atmospheric CO_2 in e-fuels production, the food industry, and microalgae production reduces reliance on fossil fuel-derived CO_2. Among DAC technologies, solid amine sorbent-based adsorption shows promise. Testing sorbents and processes under real-life conditions is crucial for performance evaluation and further development.

A pilot DAC unit with a 10 kg CO_2/day capacity, featuring a circulating sorbent system, was designed, and constructed at the University of Twente (UT). Lewatit® VP OC 1065 is used as the adsorbent in a crossflow moving bed reactor for adsorption of CO_2. The desorption process occurs in four steps: evacuation, low-temperature desorption, high-temperature desorption, and sorbent cooling, with continuous pneumatic transport of the sorbent.

The crossflow moving bed adsorber uses warmer container air in addition to cooler ambient air to reduce water loading without significantly affecting CO_2 loading. The sequential sorbent regeneration concept enhances energy efficiency by eliminating specific heat requirements during temperature swings. Each vessel operates at a consistent temperature, improving flexibility and facilitating heat integration with available waste heat.

After commissioning and initial testing at UT in August 2022, the unit was transported to Allmicroalgae in Portugal for a demonstration campaign from September to December 2022. This study conducts a detailed analysis of the pilot's performance during its testing and demonstration campaigns. This analysis of the pilot's performance highlights DAC's potential and the necessity of optimizing energy consumption and operational reliability for scalable deployment.

During UT testing, the unit operated continuously for 7 days, producing approximately 46 kg of CO_2 with 85% purity on an average due to a product recovery section leak which was later rectified. At Allmicroalgae, the unit operated for over 1500 hours, producing approximately 250 kg of CO_2 with 95% purity on an average. The average CO_2 working capacity was 0.5 mol CO_2/kgsorbent in the first half and 0.35 mol CO_2/kgsorbent in the second half. The unit operated smoothly, except for a minor issue with the sorbent transportation system in October 2022, which was promptly resolved. The campaign concluded in December 2022.

The demonstration campaign provided insights into system performance under realistic weather conditions, energy consumption, water co-adsorption, process, and sorbent stability, and the contribution of individual processes to overall energy consumption. Pilot data identified operational challenges and energy-intensive subprocesses, exploring pathways to enhance energy efficiency and process reliability.

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Title: **[OP23]** Coprecipitation of magnetite nanoparticles using a liquid/liquid membrane Reactor

Abstract: Membrane reactors (MRs) have been introduced as an alternative to traditional precipitation processesfor synthesis of inorganic nanoparticles, such as BaSO4, ZnO, TiO_2 [1]. This is mainly due to intensified micromixing and supersaturation distribution resulting in formation of nano to micro sized particles that are narrow in size distribution [2]. In this work, the possiblity of using membrane reactors for synthesis of magnetite nanoparticles (MNPs), the magnetic properties of which is highly sensitive to their size [3], is investigated. For this purpose, a process is designed and will be thoroughly discussed.

$FeCl_3$ and $FeCl_2$.4H2O salts (molar ration of 2:1) in solution are pumped into the reactor and due to a fixed pressure gradient of 0.5 bar, permeate through the pores of an assymetric tubular α-Al2O3 microfiltration membrane (100 nm pore size). The salt solution then disperses into a cross-flowing NH4OH solution (30wt% NH3 basis) through the membrane tube (permeation rate/ basic solution flowrate= 2.5) resulting in the formation of MNPs. The particles are characterized using scanning electron microscopy (SEM) and dynamic light scattering (DLS), the preliminary results of which are presented in Figure 1 and Figure 2. SEM results show successfully produced spherical shaped MNPs as small as 14.6 nm. However, the particles tend to agglomerate due to both van der Waals and magnetic forces [4]. DLS results shows the particles size distribution of these agglomerates, the average size of which is 80.4 nm.

To conclude, the possibility of producing MNPs utilizing MRs is presented. The preliminary results show the promising nature of the proposed process. Additional investigations into influential parameters (i.e., flowrate, salt concentration, and reactor configuration) in controlling the size of synthetized MNPs will be proposed. This can in turn be used to optimize the process so that a particle size distribution below 15 nm is achieved.

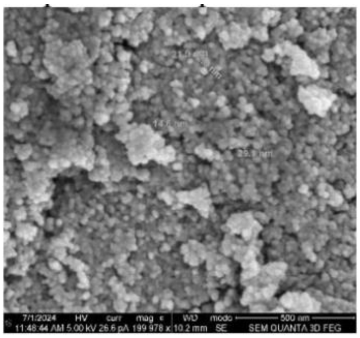

Figure 1 SEM image of the synthesized particles

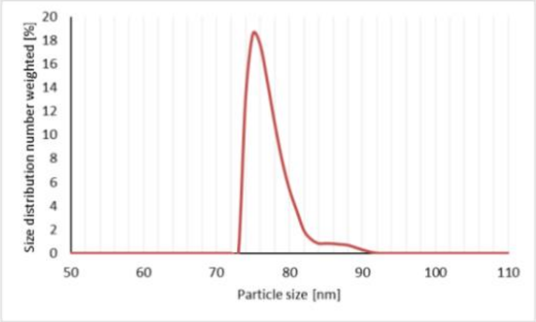

Figure 2 Size distribution of agglomerated particles

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References

[1] Jia, Z., & Liu, Z. (2013). Membrane-dispersion reactor in homogeneous liquid process. Journal of Chemical Technology & Biotechnology, 88(2), 163-168.

[2] Pellegrino, J., Schulte, L. R., De la Cruz, J., & Stoldt, C. (2017). Membrane processes in nanoparticle production. Journal of Membrane Science, 522, 245-256.

[3] Leslie-Pelecky, D. L., & Rieke, R. D. (1996). Magnetic properties of nanostructured materials. Chemistry of materials, 8(8), 1770-1783.

[4] Lyklema H 2005 Fundamentals of Interface and Colloid Science ed H Lyklema vol 4 (Amsterdam: Elsevier) pp 1.1–16.

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Title: **[OP24]** Techno-economic assessment of a decentralized system for pure hydrogen production via green ammonia decomposition

Abstract: The integration of hydrogen (H_2) selective membranes into a membrane reactor (MR) is an effective strategy for recovering H_2 from ammonia (NH_3) [1]. This study compares on a techno-economic level two pathways for H_2 production through NH_3 decomposition: the conventional and the MR-assisted routes. Given the growing interest in green NH_3 for on-site production of H_2, both processes are designed at a scale of 500 kg/day of H_2 [2] with the aim to identify the cost-minimizing operating conditions in both routes, and determine if the MR-assisted process is competitive compared to the conventional one.

The conventional and the MR-assisted processes were simulated using Aspen Plus® V11 targeting the production of H_2 to be used in PEM fuel cells for both stationary applications (SA) and on-board vehicle applications (VA). Simulations were carried out for different operating conditions of the conventional process to identify the operating conditions that minimize the cost of H_2 (COH) produced. Since the MR allows to achieve improved conversion under comparable or lower temperatures compared to a conventional reactor, simulations were then carried out for the MR-assisted process operating the reactor at the same pressure of the optimized conventional process, but at a temperature of 50 °C lower. The two routes were then compared, both from technical and economic perspectives. The reactor operating conditions that minimize the COH in the conventional process are 450 °C and 5 bar. Thus, the MR-based process was designed at a similar pressure selecting a temperature of 400 °C. While a maximum conversion of 97.8% can be achieved in a conventional reactor at 450 °C, the use of a MR allows for NH3 conversion >99% even when operating at a 400°C. While this leads to improved cold gas efficiencies, the fact that the MR-assisted process is optimized upon the utilization of a vacuum pump at the permeate side leads the MR-assisted process to display a lower overall efficiency compared to the conventional system. From an economic point of view, in facilities targeting the production of H_2 for VA, the COH in the conventional process was found to be 7.15 €/kg, while the MR-assisted process had a COH 2.8% lower, at 6.95 €/kg. Conversely, the use of a MR does not bring any economic advantage for SA. The techno-economic assessment indicates that H2 recovery from green NH3 using MRs could be achieved at lower costs than benchmark technologies, indicating significant potential for MR technology in advancing energy system decarbonization.

References

[1] V. Cechetto, L. Di Felice, and F. Gallucci, “Advances and Perspectives of H2 Production from NH3 Decomposition in Membrane Reactors,” Energy & Fuels, Jul. 2023.
[2] C. on A. and S. for F. H. P. and Use, “The Hydrogen Economy: Opportunities, Costs, Barriers, and R&D Needs,” United States, 2004.

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Title: **[OP25]** The shape-dependent activity of Pd/CeO_2 nanorods, nanocubes, and nano-octahedrons on lean methane oxidation

Abstract: Stringent regulations aimed at significantly reducing emissions of harmful and greenhouse gases (GHG) are driving a transformation in the maritime industry. The shift from heavy fuel oil (HFO) to liquified natural gas (LNG) as a maritime fuel can lower emissions of SO_2, NOX, CO_2, CO, and toxic particles [l]. However, this transition results in a fivefold increase in methane emissions1, which is problematic due to the high global warming potential (GWP) of methane of 37±10 over a 100-year horizon [2]. Oxidizing unburnt methane using palladium-based catalysts presents a promising solution for mitigating GHG emissions in LNG engines, as these catalysts achieve high conversion rates at low temperatures and short contact times [3]. Enhancing conversion at low temperatures can be achieved by using high oxygen mobility supports like CeO_2, which increase the activity of oxidation catalysts [4]. Different CeO_2 morphologies generate various facet terminations, influencing the Pd oxidation state and CeO_2 reducibility [5]. Although this concept has been previously applied to other reactions, the impact of support faceting on lean methane oxidation remains underexplored. This study investigates the influence of different CeO_2 support shapes on the activity of lean methane oxidation Pd-based catalysts.

Characterizations using BET indicate that CeO_2 nanocubes exhibit the highest surface area and the greatest concentration of oxygen vacancies (characterized by XPS and Raman spectroscopy). TEM characterizations showed that Pd particle sizes on Pd/CeO_2 nanorods have an average of 5.2 nm, while 6.0 nm were identified for Pd/CeO_2 nano-octahedrons, and 6.6 nm were observed on Pd/CeO_2 nanocubes. The similar particle size of the catalyst is important as this reaction is structure-sensitive. The addition of Pd slightly increases the surface area and reduces CeO_2 crystallite size. All catalysts show a higher concentration of oxygen vacancies compared to their supports, suggesting that the addition of 0.5 wt.% Pd promotes the formation of Ce^{3+}. Light-off curves demonstrate that the dilutant is largely inactive, with support activity increasing in the order: CeO_2 nanorods > CeO_2 nano-octahedrons > CeO_2 nanocubes. For all supports, activity increases following Pd impregnation, with Pd/CeO_2 nanorods exhibiting significantly higher activity than other shapes.

The superior performance of nanorods is attributed to their higher concentration of oxygen vacancies due to the specific facet termination of (110) (determined using TEM), bulk oxidation of Pd (characterized by XPS), larger surface area, and greater acidity (characterized by ammonia TPD).

References

[1] J. Hua, Y. Wu, H. L. Chen. Transp Res D Transp Environ 2017, 52, 254–276.
[2] R. G. Derwent. Atmosphere (Basel) 2020, 11, 5, 486.
[3] Z. Li, G. B. Hoflund. Journal of Natural Gas Chemistry 2003, 12, 153–160.
[4] T. Sakpal, L. Lefferts. Journal of Catalysis 2018, 367, 171–180.
[5] S. Colussi, P. Fornasiero, A. Trovarelli. Chinese Journal of Catalysis 2020, 41, 6, 938–950.

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Title: **[OP26]** Integrated process development for the conversion of lignocellulosic biomass to ethylene glycol

Abstract: Lignocellulosic biomass, a sustainable and abundant source of saccharides, can be efficiently converted to ethylene glycol (EG) via catalytic hydrogenolysis using heterogeneous Raney- Ni and homogeneous WOx catalysts [1,2]. This study explores using de-ashed but non-delignified lignocellulosic biomass as feed, shifting from water-based to organic-rich solvents to prevent lignin repolymerization and reduce equipment and catalyst fouling [1].

The use of organic solvents significantly improves lignin solubilization, reducing fouling risks (Fig 1-left). However, it increases WOx co-catalyst precipitation (from 70 wt% in water to an average of 83 wt% in organic solvents) and decreases glycol yield (from 30 wt% in water to an average of 20 wt% in organic solvents, with a peak of 25 wt% when using 1,4- BDO). This precipitation issue is somewhat mitigated under semi-batch operations, where the build-up of glycols seemed partly resolubilize precipitated WOx species.

The study also observed that catalysts activity remained constant over up to four cycles, as indicated by steady yields of EG, sugar alcohols (mannitol and xylitol), and glycerol, while propylene glycol (PG) yield increased cycle by cycle (Fig 1 - right). No significant hydrogenation catalyst poisoning by liberated lignin or lignin repolymerization was noted, contrary to previous studies [1].

The study also observed that catalysts activity remained constant over up to four cycles, as indicated by steady yields of EG, sugar alcohols (mannitol and xylitol), and glycerol, while propylene glycol (PG) yield increased cycle by cycle (Fig 1 - right). No significant hydrogenation catalyst poisoning by liberated lignin or lignin repolymerization was noted, contrary to previous studies1. In search for simpler and cheaper pre-treatment for producing cellulosic glycols, we show the possibility to use non-delignified biomass by (1) using organic co-solvents and (2) moving from batch to semi-batch experiments, one step towards the continuous stirred tank operation commonly used in industry.

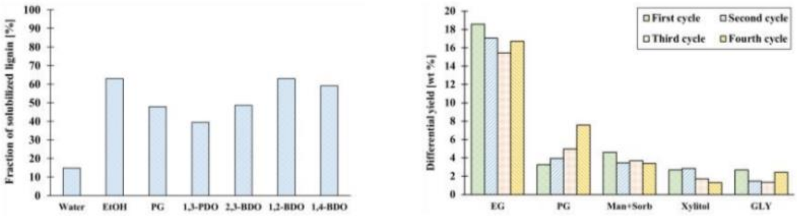

Figure 1. Left - Percentage of lignin extracted from the feed and solubilized during the reaction. Right – Differential product yield for each cycle (EG = ethylene glycol, PG = propylene glycol, Man = mannitol, Sor = Sorbitol, GLY = glycerol).

References

[1] T.D.J. te Molder, S.R.A. Kersten, J.P. Lange, M.P. Ruiz; Ind. Eng. Chem. Res. 2021, 60, 7043
[2] T.D.J. te Molder, S.R.A. Kersten, J.P. Lange, M.P. Ruiz; Ind. Eng. Chem. Res. 2021, 60, 13515

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Title: **[OP27]** Morphology controlled ceria catalysts for reverse water gas shift reaction (RWGS)

Abstract: Ceria (CeO_2) has a stable fluorite lattice structure that allows it to easily transition between Ce^{4+} and Ce^{3+} states, making it a widely used catalyst [1, 2] with exceptional oxygen storage capacity (OSC). The concentration of oxygen vacancies within CeO2, as indicated by the ratio between defect-induced band intensity (ID) and F_{2g} band intensity (IF_{2g}), follows a specific order: CeO_2 rods > CeO_2 cubes > CeO_2 octahedra. Thus, modifying the catalyst shape is an effective strategy for tuning the reactive crystal planes on the ceria surface, offering a novel approach to developing advanced catalytic materials for the reverse water gas shift (RWGS) reaction [3]. The RWGS reaction ($CO_2 + H_2 \rightarrow CO + H_2O$) converts CO_2 into CO, which serves as a fundamental building block for a variety of valuable chemicals and fuels [4]. We synthesized ceria with different morphologies, doped Ni on them and tested under different reaction conditions. Our results show that catalytic doping of Ni on ceria nanorods effectively boosts the RWGS process [Figure below].

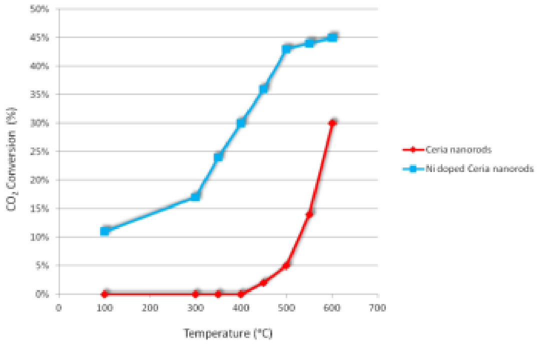

Figure - Temperature-programmed RWGS reaction over Ceria nanorods and Ni doped ceria nanorods. ($CO_2:H_2 = 1:2$)

References

[1] N. R. Shiju, Size matters: the role of metal-support bonding in controlling the particle size of ceria supported transition metal catalysts, ChemCatChem, 3, 112-114, 2011

[2] E. V. Ramos-Fernandez, N. R. Shiju*, G. Rothenberg, Understanding the solar-driven reduction of CO_2 on doped ceria, RSC Adv., 4 (32), 16456–16463, 2014

[3] M. Ronda-Lloret, L. Yang, M. Hammerton, V. S. Marakatti, M. Tromp, Z. Sofer, A. Sepúlveda-Escribano, E. V. Ramos-Fernandez, J. J. Delgado, G. Rothenberg, T. R. Reina, N. R. Shiju, Molybdenum oxide supported on Ti_3AlC_2 is an active reverse water–gas shift catalyst, ACS Sustainable Chem. Eng., 9 (14), 4957-4966, 2021.

[4] T. Mathew, N. R. Shiju, Survey of heterogeneous catalysts for the CO_2 reduction to CO via reverse water-gas shift, Chapter in the book ‘Engineering solutions for CO_2 conversion’ ISBN: 978-3-527-34639-4, Wiley, March 2021.

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Title: **[OP28]** Enhancing Methane Oxidation in Maritime Engines: A Numerical Study of Pre-Reactor Temperature Control

Abstract: Maritime transport is the backbone of global commerce, but due to the high volume of merchandise involved, it is also a major polluter. In a carbon-zero future, developing new technologies is mandatory to maintain the competitiveness of naval transportation while maximally reducing greenhouse gas (GHG) emissions, which are mainly created during fuel combustion. One of the more important pollutants is methane slip, which results from incomplete combustion in the engine. Eliminating it has proven difficult due to the complexity of natural gas combustion and its interaction with the engine's combustion chamber.

One promising alternative to reduce these emissions is to place a methane oxidation reactor downstream of the engine. By using a suitable catalyst, the reactor oxidizes methane into carbon dioxide and water. In industry, this reaction is often realized in monolithic reactors because of their high surface reaction area and low pressure drop. While this process may seem straightforward, its complexity and inefficiency increase as the water content in the processed gases rises. This is a significant issue because combusting any fuel with hydrogen molecules naturally creates water, resulting in decreased performance of the methane oxidation reactor and subsequently in higher emissions.

One way to address this and improve the performance of the methane oxidation process is to control the temperature before the reactor. This isolates the reactor's operation from the engine exhaust temperature. By controlling the temperature, we can select the best setting for the oxidation reactor based on the inlet composition, thereby decreasing methane emissions. Considering this, this study presents three different approaches for controlling the gas temperature before the reactor. The first one is using a natural gas burner to reach the desired temperature. The other option is switching the fuel from methane to hydrogen, thus reducing carbon dioxide emissions. The last option relies on using the ship's excess electricity to increase the gas temperature via an electrical resistance heater. For the first case, the model will find the optimal operating point that minimizes additional carbon dioxide emissions from the additional combustion process while maximizing the gas temperature before the reactor. Similarly, for the hydrogen case, the model will determine the minimum hydrogen flow rate required for the combustion process while maximizing the inlet temperature at the methanation reactor. Therefore, this work presents a numerical framework for evaluating the presented scenarios. For hydrogen and natural gas combustion, a combustor modeled as a well-stirred reactor was used after employing appropriate reaction mechanisms from the Cantera library. For the methane oxidation reactor, a monolith design was chosen and simulated using an in-house numerical code developed to simulate a representative channel. This code utilizes finite differences to solve the species, momentum, and energy conservation equations for a transient one-dimensional problem. Finally, this work presents the best operational points for each alternative and discusses its energy consumption and emissions.

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Title: **[OP29]** Novel internal fin configurations for gas-liquid monolithic reactors

Abstract: Packed bed reactors are widely used in the chemical process industry to perform solid-catalyzed gas-liquid reactions and gas-liquid absorption processes. These reactors are often associated with large pressure drops, local liquid mal-distribution, and partial wetting of catalyst particles resulting in high operational costs [1]. Therefore, structured packings like monoliths are being investigated as an alternative to conventional catalyst particles. Monoliths have several advantages over conventional catalyst packings like lower pressure drop, higher mass transfer rates, shorter diffusion paths [2]. The foremost challenge is to achieve uniform gas-liquid distribution as it often governs the overall performance, i.e. conversion, yield, selectivity, etc., of multiphase monolith reactors.

Few researchers have investigated the gas-liquid flow through single capillary channels, as a representative geometry of monolith, using imaging measurements [3] and 2D simulations [4].These efforts have resulted in the identification of gas-liquid flow regimes namely, dispersed bubbly flow, slug flow, churn flow, and annular flow along with their relationship with the gas and liquid superficial velocities for a specific channel size. However, a single capillary channel cannot be considered a representative of a multiphase monolith reactor as the gas and liquid phase are not injected in individual monolith channels but are injected over the monolith using distributors like shower heads, sieve plates, spray nozzles, etc [2].

Therefore, with the aid of structure-resolved volume-of-fluid simulations, we investigate the local dynamics of gas-liquid flow through a realistic 3D monolith, by considering the effect of a liquid distributor. The effect of gas and liquid flow rates as well as the presence of internal fins on the local phase distribution and the resulting flow performance parameters is investigated. Further, we not only investigate the performance of monoliths with conventional internal fin configuration but also propose new fin configurations. We show that the local liquid distribution and the resulting flow performance in terms of liquid holdup, wetted, and interfacial area are substantially influenced by the geometrical configuration of the fin especially the corner angle and the number of corners. Both, a decrease in corner angle and an increase in the number of corners promote overall flow performance in terms of liquid holdup, wetted area, and interfacial area. Furthermore, the relationship between local flow behavior, gas and liquid flow rates, as well as the resulting overall flow performance is established and presented in the form of a flow regime map.

References

[1] Azarpour, et al., 2021. Ind. Eng. Chem. 103, 1−41.
[2] Roy, et al., 2004. AIChE J., 50(11), 2918-2938.
[3] Zhao and Bi, 2001. Multiph. Flow, 27(5), 765.
[4] Lei, et al., 2016. Catalysis Today, 276, 150-160.

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Title: **[OP30]** Calibration of pore network models via inverse gas chromatography

Abstract: Porous substrates and systems are widely utilized in process engineering, e.g. in the form of supported catalysts, filters or electrodes. Among the many attractive properties, especially their high specific surface area allows for intensified fluid-fluid, as well as fluid-solid contact. Often, the use of porous substrates is crucial for an economic process performance. However, a priori description of porous systems based on macroscopic quantities is often elusive and requires substantial trial-and-error during system development until a satisfying solution is found.

A potential alternative for this time-intensive and costly design procedure is given by the utilization of carefully calibrated models. Among those, pore network models have shown to provide an intriguing trade-off between prediction of flow-patterns and computational efficiency [1,2]. Additionally, pore network models allow for comparatively straightforward coupling with heat- and mass transfer phenomena, subsequently allowing for advanced reaction design of the study of degradation processes [3].

Nevertheless, pore network models have mainly been applied to gain qualitative understanding of the target processes, due to the high effort of calibrating those models via direct numerical simulations or 3D-resolved experiments [1]. Here, we propose an alternative, low-effort calibration of the relevant model parameters via inverse gas chromatography. There, a tracer is injected into the gas flow through the porous media, subjected to adsorption at the internal surface and finally a response signal is acquired. This response signal is highly sensitive towards the surface properties and morphology of the investigated porous substrate. With this signal, a set of key parameters can be calibrated, i.e. effective cross section and curvatures, subsequently allowing for rapid upscaling of the target systems.

Within the presentation, we will discuss the approach, show initial results and discuss the implications for future design of processes with porous substrates.

References

[1] Fathiganjehlou et. al. Numerical and experimental study of the flow distribution inside slender packed beds of spherocylindrical particles 2024 PowTec doi:j.powtec.2023.119 103

[2] Eghbalmanesh et. al. CFD-validated pore network modeling of packed beds of non-spherical particle 2024 CES doi:10.1016/j.ces.2023.119396

[3] Moghaddam et. al. Effect of microstructures on mass transfer inside a hierarchically structured porous catalyst J. Por. Med. doi: 10.1615/JPorMedia.2024052053

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Title: **[OP31]** A coupled Local Front Reconstruction and Immersed Boundary Method for simulating multiphase flows with contact line dynamics

Abstract: Multiphase flows in the presence of complex solid geometries are encountered widely throughout industrial processes (e.g. synthetic fuel production) to intensify mass and heat transfer operations. The efficiency of these processes depends largely on the prevailing fluid dynamics regime inside the reaction vessel (e.g. trickle bed, bubble column reactor). This regime is governed by (among others) the dynamics of the three-phase (fluid-fluid-solid) contact line, which control the (de)wetting characteristics and the capillary action.

In order to study these hydrodynamic influences numerically, a method for fluid-fluid and fluid-solid interactions must be used and coupled at the three-phase contact line. Frequently, front capturing methods (e.g. Volume of Fluid or VoF) are used to present fluid-fluid interactions, but the accuracy of the interface representation is reduced due to the required reconstruction from an indicator function. Therefore, we focused on implementing the three- phase contact line dynamics for a front tracking method (the Local Front Reconstruction Method or LFRM) [1]. The fluid-solid interactions are accounted for by enforcing the no-slip boundary condition at the solid surface, which is done using the second-order implicit Immersed Boundary Method (IBM) [2]. Coupling of these methods consists of dynamically enforcing the local contact angle of the fluid-fluid interface with the solid surface.

This work describes the numerical model that is used to manipulate the fluid-fluid interface to enforce the local contact angle. The model performance is assessed using droplet spreading simulations on flat and spherical surfaces. The equilibrium droplet shape (i.e. the radius, height and interface outline), interfacial pressure difference, surface tension force and spurious currents are compared to analytical solutions and literature standard front capturing methods. The results show an excellent match with the analytical solutions with error margins below 1% for the interfacial shape and pressure difference of almost all cases, as well as error norms in the order of 10^{-4} for the surface tension force and spurious currents. These error values are lower than for state-of-the-art front capturing models [3,4]. Furthermore, the displayed extended functionality of the model to solid surfaces described by a surface mesh enables its use in more complex geometries without analytical representation.

References

[1] S. Shin, I. Yoon, and D. Juric. “The local front reconstruction method for direct simulation of two-and three-dimensional multiphase flows”. In: Journal of Computational Physics, vol. 230.17 (2011), pp. 6605–6646.

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Title: **[OP32]** Pressure drop of single- and two-phase flows in single pellet string microreactors: the influence of wall effect

Abstract: Micro-packed beds (μPBs) are promising for achieving process intensification of heterogeneously catalyzed reactions because of their distinctive advantages, including enhanced heat/mass transfer, precise parameter control, and easy scale-up. The single pellet string microreactor (SPSM) represents a type of μPBs with a reactor-to-particle diameter ratio (*D/d*) spanning from 1 to 1.867 [1]. In contrast to common μPBs, the SPSM exhibits relatively simple flow regimes due to its regular and repeatable packing configuration. The small D/d ratio in the SPSM can lead to the improved radial heat transfer in the bed. Besides, the absence of a core bed therein is conducive to catalyst wetting, making it appealing for optimizing catalyst performance and conducting catalyst screening/testing.

In this study, the single- and two-phase hydrodynamics of SPSMs have been characterized experimentally. First, single-phase (water or N_2) flow in polymeric capillary microreactors (D = 0.5-1.6 mm) packed with spherical glass beads (d = 400-1000 μm) was investigated. The influence of fluid flow rate, microreactor diameter and particle size on the obtained pressure drop data was revealed. Based on the experiment data, the applicability of typical literature pressure drop correlations was examined, revealing poor consistency. Consequently, further model modification, particularly to account for wall effects, was identified. The universally applied Ergun equation coupled with a hydraulic diameter correction term (including the contribution of wall surface area) was proven to render a good prediction accuracy of the current data.

Subsequently, experiments of two-phase (N_2-water) flow were performed in the above SPSMs. A high-speed camera was applied to capture the flow pattern within SPSMs and slug flow regime was observed. For further understanding, additional comparison with two-phase flow in empty microreactors was conducted. A similarity was found between slug flow in SPSMs and empty microreactors. Regarding pressure drop, a modified correlation has been proposed to describe the two-phase flow data, based on the understanding of single-phase hydrodynamics in the SPSM and a proper inclusion of gas-liquid interaction term.

The findings of this research offer valuable insights for designing and operating the SPSM, such as optimized energy consumption and favorable operational windows. Additionally, these results shed light on the internal flow mechanisms within μPBs, providing guidelines for their potential use in efficient chemical synthesis or catalyst screening.

References

[1] T. Bauer, S. Haase, and R. Lange, Chemie Ingenieur Technik, 81 (2009) 989-994.

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Title: [**OP33**] Systematic evaluation and optimization of low-carbon technologies for Colombian oil refineries' decarbonization

Abstract: Climate change, driven by increased greenhouse gases concentration in the atmosphere like CO_2 from burning fossil fuels, affects both Colombia and the world. In 2010, it caused economic losses in Colombia amounting to 2.2% of GDP. Climate change also strains public health, increasing diseases like dengue and Zika, and affects electricity generation by reducing hydroelectric production (Ministerio de ambiente y desarrollo sostenible, 2016)

This research employs system optimization to assess both short and long-term time frames for achieving Ecopetrol's committed CO_2 emission reduction goals (scopes 1 and 2). Ecopetrol is the Colombian oil and gas state-owned company. To analyze the effectiveness of the proposed technologies, two Colombian refineries are used as a case study: a medium-complexity and a high-complexity refinery. The study aims to determine if the level of complexity significantly influences the outcomes.

The technologies were selected based on technical, economic, environmental, and deployment criteria and the information obtained by conversation with experts. For the short-term horizon (2030), the selected technologies included low-carbon H_2 produced from Steam Methane Reformer with CCS, and H_2 produced from renewable electricity sources. For the long-term horizon (2050), the chosen technologies are biomass gasification, and naphtha reforming for H2 production with CCS; and CCS for fossil fuel combustion.

Second, gathering data using on-site company data (e.g., yields, mass and energy balance, operational cost), information from scientific and industrial publications, and insight gathered from expert interviews. Third, system analysis and optimization were performed using Linny-R, a mixed integer linear programming software package developed by TU Delft (Bots, 2023).The objective function aims at cost minimization with a cap on CO_2 emissions targets, resulting in the maximizing of total cash flow.

Two scenarios were run in the model: First, hydrogen demand (feedstock and feedstock+ alternative fuel), and the second CO_2 emissions target (with or without)

Furthermore, a sensitivity analysis was conducted to assess the impact of key parameters such as natural gas price, CO_2 market price, and renewable electricity price.

The results indicate that achieving long-term CO_2 neutrality is feasible by using low-carbon hydrogen (H_2) and carbon capture and storage (CCS) for flue gases. However, the approach to decarbonizing direct and indirect CO_2 emissions varies significantly between refineries with different complexity levels. The sources and contributions to CO_2 emissions inventories differ, and the productive processes exhibit varying degrees of interaction and integration. Additionally, the findings reveal that refinery complexity influences decarbonization pathways. High-complexity refinery predominantly uses low-carbon H_2 as feedstock, whereas medium-complexity refinery employs a combination of carbon capture and low-carbon H_2 as an alternative fuel.

Finally, the results of this study can serve as a guide for the decarbonization of oil refineries with similar complexity worldwide. This can help inform future investment decisions and strategic planning in the pursuit of CO_2 neutrality.

References

[1] Bots, P. (2023). Linny-r (v1.9.3). https://sysmod.tbm.tudelft.nl/linny-r/docs/

[2] Ministerio de Ambiente y Desarrollo sostenible. (2016). El Acuerdo de Paris, así actuará Colombia frente al Cambio Climático (1a ed.). WWF-Colombia.

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Title: **[OP34]** Energy and Exergy Analysis of a Coupled Dark Fermentation and Microbial Electrolysis Process for Sustainable Hydrogen Production

Abstract: This study simulates the coupling of dark fermentation and microbial electrolysis cells (MECs) to optimize biohydrogen production from vinasse, a byproduct of ethanol production, and glycerol, a byproduct of biodiesel production [1][2]. Dark fermentation breaks down organic substrates into hydrogen and volatile fatty acids [1][3], while MECs convert these byproducts into additional hydrogen with a small electrical input [2][3]. The coupling of these technologies enhances hydrogen yields and improves substrate utilization [2][3].

The simulation focuses on optimizing substrate concentration and operating conditions for co-processing vinasse and glycerol [1]. Vinasse serves as an abundant substrate for microbial activity [4][5], while glycerol provides an additional carbon source. Coupling dark fermentation with MECs further boosts hydrogen recovery, utilizing residual compounds from fermentation [2][3].

Energy and exergy analyses were conducted to assess system performance, providing a comprehensive understanding of how different factors impact the efficiency of the coupled process [1] [4]. A Monte Carlo simulation analyzed the influence of glycerol composition on energy and exergy performance, offering insights into process variability and robustness under a range of conditions [1]. The energy analysis revealed MECs achieve up to 91% hydrogen capture, though challenges like scaling and low reaction yields reduce overall efficiency. Exergy analysis identified areas for energy recovery, highlighting the potential for improved system efficiency by minimizing irreversibility and optimizing energy utilization within the process [4].

Despite these promising results, scalability and operation present challenges [1]. However, this coupled system shows potential for advancing waste-to-energy technologies and supporting the circular economy through sustainable biohydrogen production from industrial waste streams [2].

References

[1] R. Gong and B. H. Lunelli, "Exergy Analysis of Biogas Production from Sugarcane Vinasse".
[2] P. Srivastava, et al. "Coupling dark fermentation and microbial electrolysis cells for higher hydrogen yield: Technological competitiveness and challenges".
[3] Y. Lo, et al. "Dark fermentative hydrogen production with crude glycerol from biodiesel industry using indigenous hydrogen-producing bacteria".
[4] E. Carrilho, et al. "DESTINATION OF VINASSE, A RESIDUE FROM ALCOHOL INDUSTRY: RESOURCE RECOVERY AND PREVENTION OF POLLUTION".
[5] R. Haron, et al. "Conversion of crude glycerol to biohydrogen by locally isolated Klebsiella pneumoniae via dark fermentation".

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Title: **[OP35]** Experimental investigation on the hydrodynamics of a conical bubbling fluidized bed with a novel gas distribution system

Abstract: Many large-scale industrial processes, especially chemical engineering applications, widely employ fluidized beds. The hydrodynamic characteristics of gas-solid or liquid-solid interactions play a key role in the optimal functioning of a fluidized bed reactor. Numerous experimental and numerical studies on the hydrodynamics of cylindrical beds under cold flow conditions exist in the literature. However, conical fluidized beds are gaining attention as they offer several advantages over cylindrical fluidized beds such as operation with comparatively wide particle size distribution and smooth operation with a deep bed.

Therefore, the present work focuses on the experimental investigation of hydrodynamics of a conical, nitrogen-blown bubbling fluidized bed using a number of different bed materials. A novel gas distribution system employing high velocity jet nozzles at different bed heights instead of a conventional distributor plate at the bottom of the bed is used. The pressure drop across the bed and bed expansion height are measured during the experiments. These measurements provide valuable insights into the hydrodynamics of the fluidized reactor bed under consideration. Further, three-dimensional CFD simulations of the reactor bed for various operating conditions are validated with the experimental results.

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Title: **[OP36]** Photon flux and effective optical path length determination for continuous-flow photoreactor design through radiometry, chemical actinometry and ray-tracing

Abstract: Photocatalysis for small molecule activation has seen significant advancements over the past years[1], yet its scale-up remains challenging due to light attenuation effects[2]. A promising advancement lies in the use of high light intensities paired with continuous-flow reactor technology. For this, a deep grasp of photon transport phenomena is essential, typically demanding resource-intensive experiments. Our innovative workflow to photochemical reactor setup characterization addresses this by starting with radiometric light source analysis and translating this into 3D light source and reactor simulations for photon flux and effective optical path length determination[3].

This strategy decouples photon flux and pathlength determination, substantially curtailing experimental necessities. The workflow proves versatile across various reactor systems, simplifying intricate light interactions into a single one-dimensional parameter, i.e., the effective optical pathlength. Combined with the photon flux, this parameter effectively characterizes photochemical setups, irrespective of scale, light intensity, or photocatalyst concentration. Employing radiometry further offers insights into light source positioning and reactor design, obviating the need for repeated chemical actinometry measurements due to light source degradation, or exchanging it with a light source of the same manufacturer. This way light source models can be applied using varying spectral distributions, radiant powers or even reactor models.

This latter point is of interest for modular and versatile reactor design, easing the transition from batch to microflow operation, which is currently being investigated in our group. The simulation method is being applied to novel open-source 3D-printed reactor design for reproducible photochemistry in one batch and two different micro-flow photoreactor designs, for optimal photon-usage and irradiation characterization[4].

References

[1] L. Buglioni, F. Raymenants, A. Slattery, S. D. A. Zondag, T. Noël, *Chem. Rev.* **2022**, *122*, 2752–2906.

[2] S. D. A. Zondag, D. Mazzarella, T. Noël, *Annu. Rev. Chem. Biomol. Eng.* **2023**, *14*, 283–300.

[3] S. D. A. Zondag, J. H. A. Schuurmans, A. Chaudhuri, R. P. L. Visser, C. Soares, N. Padoin, K. P. L. Kuijpers, M. Dorbec, J. van der Schaaf, T. Noël, *Nat. Chem. Eng.* **2024**, DOI 10.1038/s44286-024-00089-3.

[4] T. M. Masson, S. D. A. Zondag, J. H. A. Schuurmans, T. Noël, *React. Chem. Eng.* **2024**.

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Title: **[OP37]** High yielding conversion of xylose to furfural via boronate esters

Abstract: Recent studies at the University of Twente have identified a new way of producing furfural from diluted xylose with high yield and low energy requirement using a boronate ester intermediate. [1] As xylose can readily be obtained from lignocellulosic biomass, and furfural is a proven, versatile platform chemical, this new route can play an important part in transitioning the fuel and chemical industry from oil-based to bio-based. [2]

This new method boasts a 80 % selectivity, compared to the 50% of traditional methods. To achieve this, xylose is not directly dehydrated with sulfuric acid, but first converted to an ester with an aromatic boronic acid. This esterification is selective for xylose, compared to other sugars, and produces an apolar xylose-diboronate ester, which allows for a selective extraction of xylose from aqueous media. This extraction has been proven to selectively extract xylose from a bagasse acid hydrolysate, with minimal extraction of contaminants or losses of boronic acid. Up to 90 % of xylose can be recovered effectively in three equilibrium stages. [3]

Subsequently, the ester is hydrolyzed to produce furfural at 80% selectivity. This is done at elevated temperatures and by contacting the organic xylose boronate ester solution with an acidic, saline water solution. This hydrolyses the ester, releasing free xylose. Owing to the low concentration of xylose in equilibrium with its boronate ester, the selectivity towards furfural is improved. This is also helped by the in-situ extraction of furfural to the organic phase, preventing side-reactions in the aqueous phase. The boronic acid that is released during the hydrolysis has also been re-used to extract xylose, proving that the boronic acid can be re-used through the cycle of extraction and hydrolysis. [4]

References

[1] L. Ricciardi, W. Verboom, J. P. Lange, and J. Huskens, “Synergic Effects of Boronate Diester Formation and High-Ionic Strength Biphasic Operation on Xylose-to-Furfural Selectivity,” ACS Sustain Chem Eng, vol. 10, no. 11, pp. 3595–3603, Mar. 2022, doi:10.1021/acssuschemeng.1c08265.

[2] J. P. Lange, E. Van Der Heide, J. Van Buijtenen, and R. Price, “Furfural-A promising platform for lignocellulosic biofuels,” ChemSusChem, vol. 5, no. 1. Wiley-VCH Verlag, pp. 150–166, Jan. 09, 2012. doi: 10.1002/cssc.201100648.

[3] P. J. van der Wal, S. R. A. Kersten, J.-P. Lange, and M. P. Ruiz, “Process Development on the High-Yielding Reactive Extraction of Xylose with Boronic Acids,” Ind Eng Chem Res, vol. 62, no. 20, pp. 8002–8009, May 2023, doi: 10.1021/acs.iecr.3c00364.

[4] P. J. van der Wal, J. P. Lange, S. R. A. Kersten, and M. P. Ruiz, “Kinetics of Furfural Formation from Xylose via a Boronic Ester Intermediate,” ACS Sustain Chem Eng, Feb. 2023, doi: 10.1021/acssuschemeng.3c07390.

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Title: **[OP38]** Catalytic upgrading Kraft lignin pyrolysis bio-oil: effect of process parameters and sulfur content

Abstract: The importance of biomass as an alternative fuel source has gained attention in recent years. Kraft lignin (KL) is the most produced lignin on the market and nowadays it is mainly burned for heat generation due to its chemical recalcitrance and its sulfur content [1-3]. Pyrolysis is a powerful methods used to produce bio-oil consisting of valuable compounds from the lignin polymer degradation. After pyrolysis, sulfur is present in all the different products in the form of H_2S and thiols in gas, disulfides and thiophenes in the liquid bio-oil, and in char residues as elemental sulfur [4]. Thus, catalytic upgrading of bio-oil must consider the sulfur tolerance of catalysts, which affects their activity. Cu/TiO_2-P25 shown promising performances for the selective demethoxylation of guaiacols [5], and its activity in presence of sulfur has been investigated in batch and continuous flow configuration.

In this work, the valorization of KL is obtained by pyrolysis at 550˚C with a continuous N_2 flow. A series of condensation steps allow the separation and the characterization of different fraction of bio-oil with GC-MS, GCxGC-MS GPC, and NMR. To study the poisoning mechanism of the catalyst with different sulfur concentrations, catalytic hydrotreatment experiments in continuous were performed using a model bio-oil feed of 4-methyl guaiacol (5 wt.% in toluene). Then, thiophene was add as an external sulfur source to reproduce the sulfur content of the bio-oil. Calculations have been made to have a model bio-oil with 0, 0.1, 1, 2 and 10 wt.% of sulfur content. The reaction was carried out in a fixed-bed stainless steel reactor, with 0.100g of Cu/TiO_2 catalyst mixed with 0.200g of SiC, and reduced in-situ for 2h at 360 °C and 6 bar, under a constant H_2. The feed was pumped then through the reactor. Samples were collected at intervals of 1h, for a total time of stream (TOS) of 8 h, and then analyzed by GC-MS. Catalytic hydrodeoxygenation of the oil in batch was performed with Cu/TiO_2 catalyst using high H_2 pressure reactor at 100 bar and 350°C.

The pyrolysis of Kraft lignin allowed to produce around 30 wt.% of bio-oil. Continuous reactor configurations exhibited a sulfur-related poisoning of the catalyst mainly affecting stabilization time of the conversion rate of guaiacol. Stabilization is reached after 4h in low-sulfur experiments (i.e.,0, 0.1%, 1%), and after 6h for high-sulfur ones (i.e., 2%, 10%). Conversion values of 4-methyl guaiacol model bio-oil reach 70%, with high selectivity towards demethoxylated products. Bio-oil hydrotreatment in continuous configuration results in similar conversions and stabilization times to the low-sulfur content experiments. In batch configuration almost 50% of guaiacols and catechols can be converted, resulting in an increase of demethoxylated products (i.e., phenols and alkyl phenols) from 7.5 to 33%, higher content of dehydroxylated aromatics and polyaromatics.

References

[1] J. Martin, ChemCatChem. 2022, 16, 253

[2] J N. Khwanjaisakun, Bioresour. Technol. 2020, 299
[3] H.A. Ariyanta, Int. J. Bio.I Macromol.,2023, 240
[4] M. Borella, Energies, 2022, 15,991
[5] H. Yang, Appl Catal A Gen.,2023 ,654, 119062

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Title: **[OP39]** Chemical recycling of HDPE and LDPE from municipal waste stream using Hydrothermal Liquefaction process

Abstract:

Plastic waste is a significant environmental issue in modern society. Traditional mechanical recycling has been addressing this problem but has intrinsic limitations: it requires cleaner feedstock and allows a limited number of cycles. Chemical recycling holds considerable potential as a supplementary method. Hydrothermal Liquefaction (HTL) is an emerging chemical recycling technique for plastics.

We studied the HTL of mixed waste containing predominantly HDPE and LDPE, from municipal plastic waste streams under high temperature and high-pressure conditions. Experiments were conducted at varying temperatures, durations, stirring speeds, water-to-plastic ratios, and plastic granule sizes. The three main product groups, gas, oil, and char were analyzed to determine their yield under different reaction conditions and to understand the composition of each phase. Results indicate that lower temperatures (around 430° C) and shorter reaction times yield higher amounts of oil and less gas. However, the oil produced is more viscous with longer carbon chains, sometimes even waxy. Conversely, higher temperatures (450 or 460° C) and longer reaction times result in less oil but shorter carbon chains and a higher proportion of aromatic compounds in the oil. The carbon chain distribution in the oil as a function of the temperature is shown in figure 1. A higher water-to-plastic ratio and lower stirring speed lead to more gas and less oil production. Plastic granule size did not significantly impact the HTL reaction outcomes.

According to our results[1], HTL shows promising potential in processing mixed municipal plastic waste streams. Different reaction conditions can be optimized for subsequent processes to produce new plastics or other valuable products. The results will be discussed in detail in the meeting.

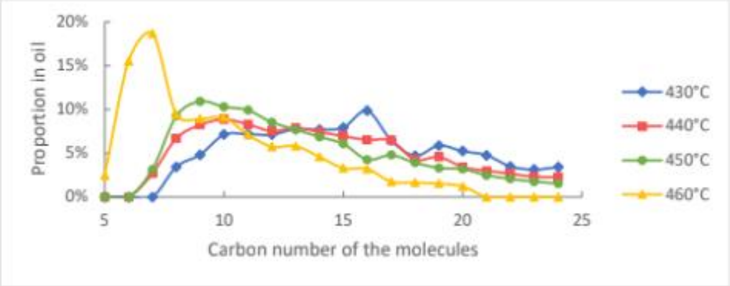

Figure 1. Carbon chain length distribution of oil at different reaction temperatures. 35 g of post-consumer HDPE plastic was ground into small pieces and liquefied with 50 ml of water for 15 minutes.

References

[1] M. J. Boel, H. Wang, A. AL FARRA, L. Megido, J. M. G. LaFuente, N. R. Shiju, Hydrothermal Liquefaction of Plastics: a survey of the effect of reaction conditions on the reaction efficiency, Reaction Chemistry & Engineering, 2024, DOI: 10.1039/D2RE00510G.

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Title: **[OP40]** The Interaction of Intrinsic Reaction and Mass Transfer in Polyethylene Pyrolysis with Reflux System

Abstract: Polyethylene, a commonly produced polymer, presents significant environmental issues due to the disposal of post-consumer waste. Pyrolysis provides an effective solution by transforming polyethylene waste into valuable chemicals and fuels. Our study aimed to explore the interaction between intrinsic kinetics and mass transfer on the yield and product distribution in polyethylene pyrolysis. We conducted experiments using both a screen heater reactor, which has minimal heat and mass transfer limitations, and a conventional semi-batch reactor at the same temperature. The results show that the intrinsic reaction rate (bond cracking) is high and consistent across the reactors. However, the mass transfer rate (evaporation) differs between reactors and can be adjusted to influence the yield and product distribution. This discovery is crucial as managing mass transfer can enhance the efficiency and selectivity of the pyrolysis process.

Additionally, we investigated how reflux affects polyethylene pyrolysis. Our findings show that the reflux temperature can be the primary factor in determining product distribution, regardless of the reactor temperature. Because the reaction rate is directly tied to the reactor temperature, higher temperatures can boost the oil production rate without greatly altering its composition. This insight is crucial for designing reactors and determining their capacity. Nonetheless, it’s important to consider the balance between increased production and the energy demand, as reflux necessitates extra heat input in the reactor.

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Title: **[OP41]** Optimizing electrochemical conversion of CO_2 to ethylene via multi-physics simulations

Abstract: The low-temperature electrochemical conversion of CO_2 to ethylene holds a great potential to defossilize a significant part of the chemical industry. Despite recent breakthroughs, the key performance indicators (activity, selectivity, durability) of this process are not yet sufficient to push the technology towards industrial implementation.

Among the various possibilities, the membrane-electrode-assembly (MEA) cell design seems the most promising to achieve higher current densities, despite new challenges arise, such as flooding of the gas diffusion electrode. Furthermore, it has been recently experimentally demonstrated that selectivity of the process can be greatly enhanced by appropriately combining two different catalysts (silver, copper) and promoting in-situ tandem reaction (CO_2->CO and then CO->C_2H_4) [1]. Nevertheless, the design parameter space is ample and further optimization of the electrochemical cell and operating conditions are still possible and necessary.

Computational modelling can support in this optimization endeavor, therefore accelerating material innovation and testing. For this purpose, a multi-physics computational model was developed at the cell-level to understand the impact of different geometrical features, material properties, and operating variables.

First, a 1D model has been developed based on existing literature [2]. The model is steady-state isothermal, focuses on the cathode region, and the GDL is assumed liquid free. Gas and liquid flow, transport of 14 species (multi-species diffusion) and 13 reactions (heterogeneous and homogeneous) are modelled in the different (porous or open channel) regions. By comparing/fitting against literature experimental data and in-house experiments, the reaction parameters (exchange current densities) are appropriately chosen.

Next, the model has been extended to 2D to capture variations of the key quantities (e.g. concentrations) along the flow direction, and crucially study the impact of spatially varying material properties (e.g. catalyst loading and composition) on the cell performance. Different parameter variations have been investigated, including gas feed composition, catalyst loading, catalyst active area, GDL porosity. The impact of these parameters on I-V curve, Faradaic efficiency, and spatial distributions of the key quantities (concentrations) will be reported, and optimal parameter combinations will be shown.

References

[1] Zhang et al. Nature Catalysis 5, 202 (2022)
[2] Weng et al. Energy and Environmental Science 13, 3592 (2020).

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Title: **[OP42]** Regeneration of Iron Powder from Combusted Iron Products by Low-Temperature Electroreduction Method

Abstract: Iron powder is a promising energy storage and carrier due to its high energy density and transportability. In the "iron fuel cycle, " energy is released by combusting iron powder, and the resulting iron oxides can be recycled into iron powder. Electrochemical reduction (electroreduction) offers advantages such as low temperature/energy consumption and direct use of renewable power without sintering particles(as in high temperatures thermochemical reduction). However, the unique characteristics of combusted iron products pose challenges for low-temperature electroreduction in an alkaline system, including the presence of various oxide phases (a mixture of magnetite, hematite, and wustite), larger particle sizes (30-80 μm) compared to hematite powder used in literature, and the presence of unburned iron particles. To address these challenges, experiments are carried out using a parallel plate electrode immersed in a suspension of combusted iron powder-aqueous sodium hydroxide electrolyte (18M, 110° C) inside a beaker glass surrounded by circulating calorific oil. This study demonstrates, for the first time, the feasibility of electrochemically regenerating metallic iron from combusted iron products with a promising current efficiency of 82% and low electrical energy consumption (<5 kWh/kg-Fe), achieved in j=1000 A/m^2 and 10 wt% combusted iron mass fraction. However, higher current densities affect lower current efficiency due to massive hydrogen evolution reaction (HER), in line with the previous studies. Generally, the deposits appear brittle, moss-like, and porous/rough, allowing easy harvesting or iron deposits. The SEM images show that the deposits predominantly consist of needle-like dendritic microparticles, ranging between 10-60 μm. Nevertheless, improvements in the rinsing technique are necessary to fully remove sodium content from the deposits, thereby achieving high-purity deposits. These results underscore the potential of this reduction technique to sustain the iron fuel cycle and promote its adoption as a CO_2-free energy carrier.

References

[1] P. Debiagi, et al., 2022, Renewable and Sustainable Energy Reviews, 165, 112579
[2] A.I. Majid, et al., 2023, Electrochimica Acta, 467, 142942
[3] A.I. Majid, et al., 2022, ECS Meeting Abstract, MA2022-02 937
[4] A. Allanore et al., 2010, J Appl Electrochem, 40, 1957-1966
[5] A.I. Majid, et al., 2024, Chemical Engineering Science, 291, 119931

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Title: **[OP43]** Salt accumulation in bipolar membranes reduces power in acid-base flow batteries

Abstract: **Introduction.** Increasing share of renewables is only possible with widespread adoption of large-scale energy storages. Redox flow batteries (RFBs) provide a great flexibility in adjusting an energy storage parameters for a customer needs, but their high cost limits their further development. Acid-base flow batteries (ABFBs) are meant to mitigate this issue as they store energy using abundant and environmentally benign solutions of acids and bases.

For almost a decade of development[1], researchers achieved impressive results in optimizing battery performance and understanding underlying processes occur in ABFBs. Nevertheless, a lot of work to be done to make this technology competitive with more mature RFBs, particularly in terms of performance stability. Improvement of cycling stability is especially challenging because the very concept of energy conversion makes ABFBs prone to crossover of salt ions between the battery compartments. Previous experimental studies showed the detrimental effect of crossover including reduced coulombic[2] and voltaic[3] efficiencies. To better understand the above negative effects, in this work we aimed at investigating crossover pathways in ABFBs and analyzing detrimental effect of background salt in acid and base solutions on a bipolar membrane performance.

Experimental section. First, we analyzed crossover pathways in ABFBs and measured salt ions fluxes though a bipolar, cation- and anion-exchange membranes using H-cell filled with two electrolytes solutions. Then, we measured polarization curves (under reverse and forward biases) of a bipolar membrane, which uses acid and base solutions of various composition from both sides of the membrane. The electrolytes differ in acid/base concentration and type, and salt content. We used acquired data to obtain open circuit voltage (OCV), resistance and limiting currents of the membrane for a given composition of electrolytes. Moreover, we used electrochemical impedance spectroscopy at OCV, under reverse or forward biases to reveal the membrane resistance breakdown.

Results and discussion. The appearance of background salt in acid and base does not change much the membrane performance under reverse bias, while its effect for forward bias is detrimental. We state that under forward bias salt-ions compete with H^+ and OH^-, which results in salt accumulation near junction of a bipolar membrane [4]. Moreover, we revealed that anion-exchange layer of the membrane is more sensitive to crossover. As a result, one can evidence 4-fold decrease in ABFB power density when using salt-contaminated electrolytes, while adjusting the size and valence of salt ions one can affect the magnitude of this phenomenon.

References

[1] Kim, J. H. et al (2016). *Electrochemistry Communications*, *72*, 157–161.
[2] van Egmond et al (2018). *International Journal of Energy Research*, *42*(4), 1524–1535.
[3] Zaffora A. et al (2020). *Energies*, *13*(20), 5510.
[4] Pärnamäe, R. et al (2023). *Environmental Science and Technology*, *57*(26), 9664–9674.

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Title: **[OP44]** Electro-separation technologies for sustainable chemical industry: technology ranking and industrial perspectives

Abstract: Electrochemical separation technologies can be broadly defined as technology aiming to (selectively) recover or remove a target compound under the effect of an applied electric field. Such technologies are typically based on ion-conductive materials (either membranes or resins, e.g. electrodialysis and electrodeionization), adsorption onto an electrode (e.g. capacitive deionization), or faradaic reactions at the electrodes to drive chemical/physical transformations in solution (e.g., electrocoagulation or electroprecipitation). Initially developed for desalination and water treatment applications, electro-separation technologies are receiving increasing attention across different sectors, with the possibility to unlock novel sustainable applications [1]. In fact, such technologies offer several advantages, i.e., modularity (ease of scale-up), flexibility (rapid ramp-up/down), mild operating conditions, enhanced mass transfer given by electric field, easy reaction kinetics control and metering of products.

In this contribution we will present the results of our analysis on 15 different electro-separation technologies, including a qualitatively ranking based on a list of technical and environmental key performance indicators, as well as a number of promising industrial applications (including, e.g., metal recovery, carbon capture [2], biobased downstream processing). Based on this initial ranking, we have identified the most promising electro-separation technology for each specific applications, and experimentally investigated some concepts under laboratory conditions. Finally, we will present our results of the techno- economic analysis, to assess the economic viability of each investigated concept. Notably, although energy efficiency is often mention as an advantage, our analysis shows that such statement is strictly process-dependent and therefore cannot be generalized, but CAPEX/OPEX should be estimated case by case and benchmarked against the best available thermally-driven alternative.

References

[1] Mutch, “Electrochemical separation processes for future societal challenges,” Cell Reports Phys. Sci., 3 (2022) 100844.
[2] Vallejo Castano et al., “Optimizing alkaline solvent regeneration through bipolar membrane electrodialysis for carbon capture,” Chemical Engineering Journal 488 (2024) 150870.

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Title: **[OP45]** CO$_2$-Responsive Etalon Membranes (CREM) for in-situ analysis of ocean water

Abstract: To achieve the goal of limiting global warming to 2℃ by 2050, negative emissions technologies (NETs) should be deployed to counterbalance emissions from various sectors, including energy production [1]. CO$_2$ can be captured electrochemically (fitting the electrification transition) from ocean water (Direct ocean capture, DOC). Ocean water benefits from the 150x higher CO$_2$ concentration compared to air. This technology uses controlled pH adjustments of seawater to extract dissolved CO$_2$ and restore the ocean- atmosphere equilibrium [2]. Precisely determining the ocean water composition, in particular the Dissolved Inorganic Carbon (DIC), is a prerequisite for the effective implementation of DOC. At the same time, no accurate sensors are available for in-situ DIC analysis, which is additionally challenging due to the salt matrix in ocean water. In this work, we demonstrate real-time analysis and in-situ detection of DIC in ocean water with CO$_2$-Responsive Etalon Membranes (CREM), which would facilitate the widespread adoption of DOC across diverse locations.

We fabricate microfluidic-scale chip membranes based on transparent gold coated Si3N4 membranes with etched pores of 4 μm in diameter (Fig.1). Poly(N-isopropylacrylamide) (pNIPAm)-based microgels are spin-coated, with a gold layer deposited at both sides, forming a microgel-based etalon [3] membrane. Functionalization of pNIPAm microgels with 4-vinyl pyridine (4VP) renders the microgels responsive to CO$_2$. The microgels will swell/shrink in response to the presence of the analytes leading to a peak shift in the reflectance spectrum. To fully characterize CREM, we developed a flow cell to facilitate "in- flow AFM" observations. This innovative approach allows us to examine how membranes respond and deform both topographically and mechanically, providing crucial insights int0 microgel behavior and enabling us to optimize designs for continuous DIC level monitoring in ocean water, thereby enhancing the effectiveness of DOC technologies.

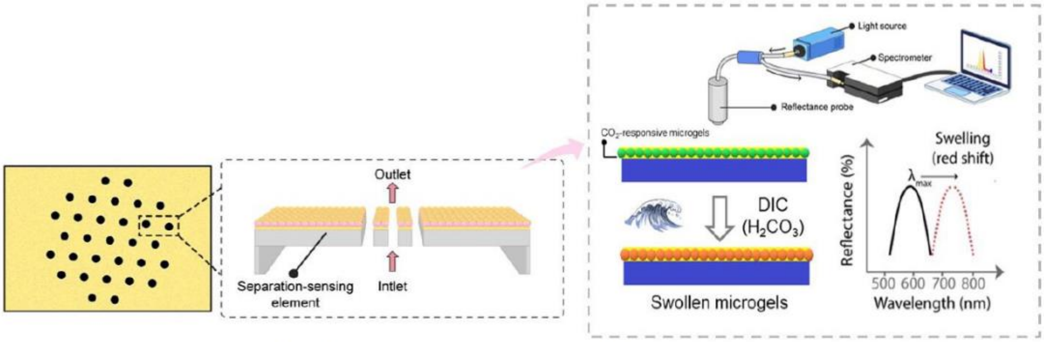

Figure 1. Working principle of CREM for DIC analysis in oceanwater.

References
[1] Smith, P., Davis, S., Creutzig, F. Nature Clim Change 2016;6, 42-50.
[2] de Lannoy, C. F., Eisaman, M. D., Jose, A. et. al. 2018;70, 243-253.
[3] Gao Y, Li X, Serpe MJ. RSC Advances 2015;5(55):44074 – 87.

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Title: **[OP46]** Development of novel polymeric precursors for the synthesis of selective carbon membranes for gas separation

Abstract: Carbon membranes (CMs) are renowned for their energy efficiency and stability in gas separation. Significant advancements have been achieved since initial trials by optimizing the parameters of the CMs fabrication process. Several studies have demonstrated that the final performance of these technologies is profoundly affected by the selection of the polymeric precursor and the carbonization temperature [1]. This research aims to explore novel polymeric precursors for synthesizing CMs, with goals including: enhancing CMs' gas separation performance to surpass the current Robeson Upper Bound [2]; shifting focus to greener, more sustainable, and less toxic raw materials through a more accurate selection of reactants and solvents, developing materials capable of achieving challenging gas separations such as CO/CO_2 or H_2/H_2O. As a first step, existing polymeric precursors were modified. The phenol-formaldehyde resin Novolac has been successfully used in previous studies for various gas separations [3], [4]. An initial attempt involved replacing the more toxic phenol with a less toxic monomer, 1,3,5-trimethoxybenzene (TMB), to study the impact of this molecule on the morphology and structure of the final CMs. The CMs obtained from the pyrolysis of this new material demonstrated competitive performance compared to Novolac-based CMs in H_2/N_2 and H_2/H_2O separations. Furthermore, investigation of another material containing imine functional groups yielded CMs with selective properties for separating H_2 from N_2, CO_2, and CH_4. Characterization techniques such as Raman spectroscopy, XPS, perm-porometry, TGA, MALDI-TOF, NMR, and SEM have been utilized and planned to elucidate performance phenomena in both current and future materials under study.

References

[1] A. F. Ismail and L. I. B. David, "A review on the latest development of carbon membranes for gas separation," J Memb Sci, vol.193, pp. 1-18, May 2001.
[2] L. M. Robeson, "The upper bound revisited," J Memb Sci, vol. 320, no. 1–2, pp. 390–400, Jul. 2008.
[3] A. Rahimalimamaghani, H. R. Godini, M. Mboussi, A. Pacheco Tanaka, M. Llosa Tenco, and F. Gallucci, "Carbon molecular sieve membranes for selective CO2separation at elevated temperatures and pressures," Journal of CO2 Utilization, vol. 68, Feb. 2023.
[4] X. Zhang, H. Hu, Y. Zhu, and S. Zhu, "Effect of carbon molecular sieve on phenol formaldehyde novolac resin based carbon membranes," Sep Purif Technol, vol. 52, no. 2, pp. 261–265, Dec. 2006.

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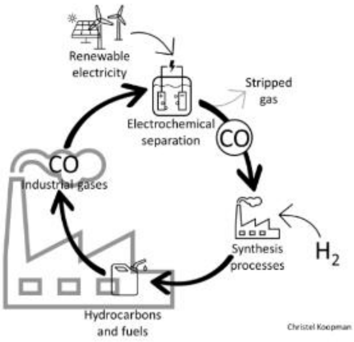
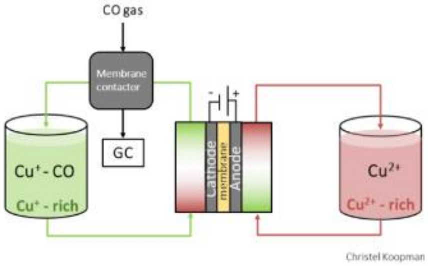
Title: **[OP47]** Electrochemically mediated separation of carbon monoxide

Abstract: Separation technologies contribute to roughly half of the energy consumption in process industry with 80% of the current separations being heat-driven.[1] To decarbonise the industry, we need to develop alternative separation technologies. Electrochemically-mediated separation can offer the efficient use of renewable electricity through targeted supply of energy to the active sites of sorption, as well as the potential benefit of operating at ambient temperatures and produce high pressure products.

We aim to develop an electrochemically driven separation process for carbon monoxide. Carbon monoxide is both an important feedstock for the production of higher value chemicals and fuels, as well as a by-product of certain industrial processes. Therefore, as part of the transition to a circular carbon economy, we aim to connect these two carbon monoxide streams. Conventional separation methods fail to efficiently separate carbon monoxide from gases such as nitrogen, which results in flaring of the carbon monoxide and thus adding to the emissions of CO_2.





Taking inspiration from haemoglobin, we propose an electrochemical separation process that leverages the affinity of transition metals, such as Fe^{2+}, to carbon monoxide. This process relies on an electro-active sorbent material, where the affinity of carbon monoxide to this sorbent material depends on the oxidation state of the material and thus allows for capture and release by potential control.

We demonstrate electrochemical separation of carbon monoxide through absorption with Fe-, Ni- and Cu-based complexes. With these materials, we obtained a proof-of-concept for electrochemical purification of 5% carbon monoxide in a mixed gas stream. Our study includes design strategies and process optimisation to improve on performance such as faradaic efficiency, capacity utilisation and product recovery. With that, we highlight the potential and challenges to separate carbon monoxide from gas mixtures via an electrochemically-mediated separation process.

References

[1] Sholl, D.S. Lively, R.P. *Nature* **2016**, 532, 435-437

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Title: **[OP48]** Advanced downstream processing for recovery of bioalcohols from fermentation broths

Abstract: Increased energy security concerns, rapid depletion of fossil carbon reserves and strict environmental constraints inevitably drive a shift toward renewable energy sources. In that respect, biotechnology has a significant potential for producing bioalcohols but is not always competitive with conventional petrochemical processes. Major drawbacks in the downstream processing after fermentation are dilute streams, low product concentrations (often < 6 wt%), by-product formation, microorganisms’ presence and azeotrope formation with water. Consequently, recovery processes are challenging and expensive (20 – 40 % of the total production costs). Therefore, this original work proposes and analyses highly advanced downstream processes for recovering different bioalcohols after fermentation.

Due to the stronger inhibitory effects on microbes, the achievable concentrations of monohydric aliphatic alcohols in the fermentation broth decrease with the increasing chain length (e.g. 6.14, 5.00, 1.61 and 0.24 wt% of ethanol, isopropanol, isobutanol and hexanol). This end-product inhibition phenomenon might be mitigated by continuously removing fermentation products from the broth in a concurrent alcohol removal and fermentation (CARAF) process. Furthermore, the initial removal should be performed without harming microbial viability. Recycling the remaining broth to the upstream process may be beneficial for avoiding biomass loss, reducing water requirements and increasing substrate-to-product fermentation yield. The compared recovery processes consist of several steps: initial removal of volatile fermentation products (heat pump-assisted vacuum distillation,[1,2]hybrid combination of gas stripping and heat pump-assisted evaporation [3] or novel pass-through distillation combined with heat pump-assisted desorber or multi-effect distillation [4]), preconcentration (heat pump-assisted distillation) and final purification (extractive distillation or liquid-liquid separation combined with distillation). According to our previous work, the total purification costs increase from 0.080 $/kg for ethanol[1], 0.109 $/kg for isopropanol [2] and 0.161 $/kg for isobutanol [3] to 0.529 $/kg for hexanol [5]. A similar trend is noticeable for the energy usage (0.960 [1], 1.348 [2], 2.018 [3] and 3.069 $kW_{th}h/kg$ [5] respectively) and the related CO_2 emissions (0.164[1], 0.221 [2],0.449[3] and 0.555 $kgCO_2/kg$ [5] respectively). However, more expensive downstream processing in the case of longer-chain alcohols is mainly due to lower concentrations in the fermentation broth and not the nature of the alcohol product. Moreover, starting from the same alcohol concentration in the broth, recovery of isobutanol and hexanol may be less expensive than the recovery of ethanol and isopropanol due to the heterogeneity of the azeotropes with water. Consequently, the performance of downstream processing is determined by achievable product concentration and not the alcohol length [5]. Lastly, this study emphasizes the importance of advanced separation and purification, based on process intensification principles, in industrial biotechnology development. In that respect, simultaneous development of upstream and downstream

processing is necessary to ensure the competitiveness and viability of industrial fermentation processes.

References

[1] Janković, T.; Straathof, A. J. J.; Kiss, A. A. Advanced Downstream Processing of Bioethanol from Syngas Fermentation. Separation and Purification Technology 2023, 322, 124320.

[2] Janković, T.; Straathof, A. J.; Kiss, A. A. Advanced Purification of Isopropanol and Acetone from Syngas Fermentation. Journal of Chemical Technology & Biotechnology 2023, 99, 714 – 726.

[3] Janković, T.; Straathof, A. J. J.; Kiss, A. A. Enhanced Isobutanol Recovery from Fermentation Broth for Sustainable Biofuels Production. Energy Conversion and Management: X 2024, 21, 100520.

[4] Janković, T.; Straathof, A. J. J.; McGregor, I. R.; Kiss, A. A. Bioethanol Separation by a New Pass-through Distillation Process. Separation and Purification Technology 2024, 336, 126292.

[5] Janković, T.; Straathof, A. J. J.; Kiss, A. A. A Perspective on Downstream Processing Performance for Recovery of Bioalcohols. Journal of Chemical Technology and Biotechnology 2024.

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Title: **[OP49]** Ferrofluidic millimeter-scale extraction systems for countercurrent slug flow liquid-liquid extraction

Abstract: The mass transfer efficiency in milli- and microfluidic liquid-liquid extractions (LLX) is typically much higher than in conventional systems, due to the small dimensions leading to a high surface to volume ratio and consequently minimal diffusion transport limitations. However, extractions in micro- and millichannels are usually performed as co-current extractions, while LLX typically benefits from countercurrent flow that facilitates multi-stage extraction in one device due to a larger driving force (1). The reason for this is that countercurrent flow at these scales is not straightforward to achieve due to the dominance of viscous and interfacial forces, as well as other operational challenges such as channel blockage because of droplet coalescence, and phase separation (2-4). The slug flow regime provides high overall mass transfer due to the continuous phase thin film between the wall and the slugs, also generating internal circulation in slugs due to shear forces that can reduce boundary layer thickness and enhance mass transport (5). This work proposes a new relatively simple concept using ferrofluids and magnetic forces to achieve slug flow countercurrent extraction process in a millichannel extractor. By applying moving permanent magnets and ferrofluid slugs, the external driving force of the magnet enables ferrofluid slugs to move against the pressure gradient. Our aim was to determine under which conditions countercurrent flow in micro- and millichannels was feasible. In order to do so, the effect of various volumetric flowrates, organic phase flowrates, and the slug flow velocity on the operational stability of this countercurrent extractor using a system of aqueous ferrofluid (AqFF) and heptane, with extraction behaviour investigated by extracting guaiacol from the AqFF to heptane. The number of theoretical stages (NTS) and the length equivalent to a theoretical stages (LETS) were determined for this system in order to quantify performance. Various operational conditions have been investigated in order to achieve the NTS above one. However, the highest NTS obtained was 0.82 ± 0.07 stages, with LETS estimated at around 31.08 ± 2.39 cm in a 25 cm channel with a 2.5 mm inner diameter. The NTS did not exceed one, likely due to channel geometry and flow condition, which caused low interfacial area and mixing efficiency. In order to increase the NTS, various system parameters may be varied, including extending the channel length or decreasing the channel diameter, or adjusting flow conditions to vary slug length. This work demonstrates that a magnetic driving force enables countercurrent LLX at millimeter channel dimensions where stable slug flow regimes can be achieved. Overall, the concept seems promising to tackle the bottleneck of countercurrent microextraction.

References

[1] C. Du et al., Sep. Purif. Technol., 295 (2022) 1-10.
[2] A. Holbach, N. Kockmann, Green Process. Synth., 2 (2013) 157-167.
[3] D. Jaritsch et al., J. Fluids Eng., 136 (2014) 1-7.
[4] Y. Liu, et al., Chem. Eng. J., 402 (2020) 1-12.
[5] C. Xu, T. Xie, Ind. Eng. Chem. Res., 56 (2017) 7593-7622.

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Title: **[OP50]** From waste to refinery – turning plastic waste into a suitable feedstock for the production of new materials

Abstract: In society, the use and disposal of plastics has increased ever since its invention. With the need for a more circular economy, the recycling of plastic waste has become a major challenge. Pyrolysis of mixed plastics has often been considered as a promising solution. This work focuses on the conversion of plastic waste to a refinery feed and particularly naphtha using pyrolysis with the intention to obtain high yields and quality. Instead of using a 'clean' feedstock, as typical done in low TRL research activities, real household plastic packaging waste (DKR 350, post-consumer-separated), obtained from a local sorting facility, was used.

The material composition of the sorted stream was determined by manual characterization and preparation was performed by shredding and agglomeration. The effect of process conditions on oil and naphtha yield were determined and optimized using a systematic experimental design approach with time (0-4h), temperature (380-450 ºC), and nitrogen pressure (up to 50 bar at room temperature). The products were characterized in detail to gain insight into the molecular composition of the oil, solid and gasses, including Simulated Distillation (Cryo-GC-FID) and elemental analysis (C, H, N, O, S) for the oil phase. It was found that a low temperature of around 380-450 ºC is the best for obtaining a high yield of naphtha range hydrocarbons (C5-C12).

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Title: **[OP51]** Induction heating with bulk inductive materials for reverse water gas shift reaction

Abstract: Induction heating is an attractive technology for reverse water gas shift (RWGS) reactors due to its advantages for efficient in-situ heat generation. This method uses electromagnetic induction to heat materials directly, which can lead to rapid and localized heating. However, one of the primary challenges associated with induction heating in RWGS reactors is achieving a uniform temperature field throughout the reaction zone. Typically, a bulk inductive workpiece is used as a heat source because traditional catalysts generate limited heat through induction heating. The distribution of the temperature field is significantly influenced by various magnetic effects, including the skin effect, slot effect, and proximity effect. These effects result in the redistribution of eddy currents within the material, leading to non-uniform heating.

In this study, we investigate the use of ferromagnetic and paramagnetic metal workpieces with various shapes and structures in both two-dimensional (2D) and three-dimensional (3D) configurations to optimize the temperature field within the reactor. By analyzing different geometries and materials, we aim to enhance the uniformity and efficiency of the heating process. The findings suggest that maximizing and closing the eddy current loops within the workpieces is crucial for achieving high energy efficiency. Among the configurations tested, double-ring workpieces have shown promising performance for the RWGS reaction at low temperatures. However, maintaining temperature control around the Curie point of iron (Fe) remains challenging, potentially due to phase transitions occurring in the material at this temperature. Materials such as iron (Fe), nickel (Ni), and stainless steel were found to be particularly effective in enhancing energy efficiency. These materials exhibit desirable magnetic properties that facilitate the generation and maintenance of strong eddy currents, thereby improving the overall heating performance. Additionally, the study explores the potential of specially designed 3D workpieces that are optimized to enhance heat transfer. These 3D configurations are tailored to create optimal loops of eddy currents, which can significantly improve the uniformity of the temperature field and the efficiency of the heating process.

Overall, this study demonstrates that the design and material composition of inductive workpieces play a critical role in the performance of induction heating for RWGS reactors. By carefully selecting and optimizing the shapes, structures, and materials of these workpieces, it is possible to achieve more uniform temperature distributions and higher energy efficiencies. This study provides valuable insights into the design principles for inductive heating systems and underscores the importance of considering magnetic effects and material properties in the development of efficient RWGS reactors.

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Title: **[OP52]** Chemical recycling of hard to recycle mixed waste plastics

Abstract: The chemical recycling via pyrolysis of mixed waste streams is challenging. One critical issue is that direct pyrolysis of this stream yields a pyrolysis oil of low quality, unsuitable for processing in petrochemical complexes, mainly due to the presence of hetero-atom containing components and other impurities.

This research shows the technological feasibility to recycle these hard-to-recycle streams into “virgin” chemical building blocks. First the waste stream is divided into two streams by means of a two-step negative NIR optical sorting to remove all (residues) but PE and PP.

The first stream, the olefin rich stream, is converted into high-quality pyrolysis oil via pyrolysis in a fluidized bed reactor. The high-quality pyrolysis oil is suitable for conversion into naphtha via catalytic hydrogenation. The naphtha can be further processed in existing naphtha crackers to produce a wide variety of petrochemicals, including ethylene and propylene.

The second stream, the olefin poor stream, is converted into mixed aromatics via Integrated Cascading Catalytic Pyrolysis (ICCP). The mixed aromatics are suitable for processing in existing aromatics plants to produce benzene, toluene, and xylenes. The elegance of the approach outlined in this research is that the complete pallet of petrochemical building blocks, olefins and aromatics, are produced from a low-quality, hard to recycle plastic waste stream, thereby proving that full circularity of all plastic waste streams is technologically feasible.

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Title: **[OP53]** Waste plastic recycling: polypropylene hydrogenolysis over Ni/Al_2O_3 catalysts

Abstract: Waste plastic recycling contributes to a circular carbon economy, and receives significant attention across academic, industrial and societal domains. Catalytic hydrogenolysis is a forefront depolymerization strategy for converting polyolefin to high-value hydrocarbon liquids. Most reported polypropylene (PP) hydrogenolysis catalysts are precious metal-based, such as Ru and Pt.[1] As such, there is an incentive to use alternative earth-abundant metal-based catalysts. Nickel-based catalysts are potentially promising replacements.[2,3] However, the use of such catalysts is still in its infancy, and systematic process studies to elucidate the relationships between catalyst activity and reaction pathways are lacking.

In this contribution, three alumina-supported Ni catalysts (15 wt.% Ni) were prepared using acidic, neutral, and basic γ-Al_2O_3 (Ni/A-Al_2O_3, Ni/N-Al_2O_3, and Ni/B-Al_2O_3, respectively) by a wetness impregnation method to investigate various reaction pathways of Ni-based catalysts for PP hydrogenolysis. The catalysts were evaluated for a representative isotactic PP at 300 °C, 30 bar for 30 h, with 5 g polypropylene and 0.5 g catalyst. The collected gas phase products ($C_{1\text{-}3}$) were analyzed by GC-TCD and liquid phase products (C_{4+}) were analyzed by GC-FID, GPC, and NMR. Remarkable differences in product distribution were observed, with Ni/B-Al_2O_3 exhibiting the highest selectivity for lighter alkanes and achieving a 31wt% yield of high-value hydrocarbons ($C_{4\text{-}20}$) and a 32 wt% methane yield, suggesting enhanced PP depolymerization rates for Ni/B-Al_2O_3. Furthermore, the liquid phase products (C_{4+}) were analyzed using NMR to reveal the main reaction pathways. The extent of the terminal demethylation including C_p-C_t bond scission and secondary C_p-C_s bond scission over Ni/B-Al_2O_3 and Ni/N-Al_2O_3 catalysts were 2.7 and 1.7 times higher than that of Ni/A-Al_2O_3 catalyst. Interestingly, the extent of internal C_s-C_t bond scission over the three catalysts was similar. These results demonstrate that PP hydrogenolysis over Ni/B-Al_2O_3 catalyst is due to more extensive terminal C-C bond scission.

Catalyst characterization studies (N_2 physisorption, XRD, TEM, ICP-OES, H_2-TPR, H_2/NH_3/CO_2-TPD, pyridine-FTIR, and XPS) were employed to identify relevant properties of the catalysts and to couple catalyst structure with performance. Notably, the cationic/metallic nickel ratio of the three catalysts was significantly different and this is most likely the cause for the differences in catalyst performance for PP hydrogenolysis.[4]

References

[1] Z. Dong, ACS Catal. 2022, 12, 14882−1490
[2] B. Vance, Appl. Catal. B: Environ. 2023, 322, 122138
[3] Z. Zhao, Environ. Pollut. 2022, 313, 120154
[4] B. Vance, JACS Au. 2023, 3, 2156-2165

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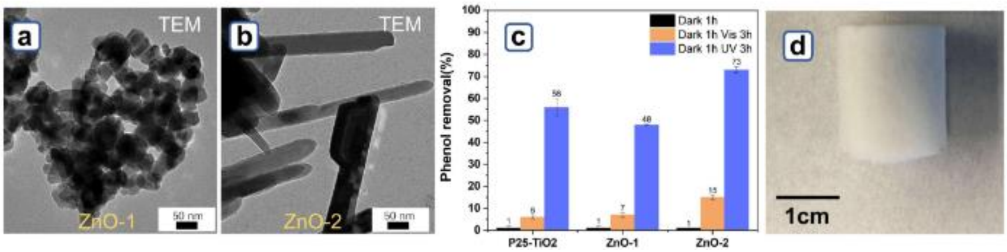
Title: **[OP54]** Batch and Continuous Degradation of Organic Pollutants in Water using Defect-Tuned Nanosized ZnO Photocatalysts

Abstract: Industrial, agricultural, and domestic activities discharge various persistent organic pollutants into the water, such as dyes, phenolic compounds, pesticides, and pharmaceuticals posing risks to the environment [1]. Effective remediation strategies are necessary, and photocatalysis is a sustainable and efficient technology that utilizes radiation (ideally solar) to mineralize organic pollutants into harmless by-products (such as CO_2 and H_2O) at ambient temperature and pressure. Zinc oxide (ZnO) is a promising semiconductor photocatalyst because of its activity under UV radiation, chemical stability, low price, and low toxicity. However, ZnO suffers from rapid recombination of the photogenerated electron-hole pairs and limited visible light utilization (wide bandgap 3.37 eV) [2].

In this study, we report the photocatalytic activity of ZnO nanoparticles prepared by tuning the type and concentration of defects through a low-cost controlled atmosphere calcination method. The photocatalytic efficiency of ZnO nanoparticles was assessed by measuring the removal of 200 ppm of selected probe pollutants in 5 ml aqueous solution with 5 mg of the photocatalyst utilizing a batch photoreactor. By tuning the contact between air and precursor, the morphology of ZnO changed from ZnO-1 irregular particles to ZnO-2 well-defined nanorods (see TEM in Fig. a and b), with increasing surface defects and decreasing bulk defects, as evidenced by characterization with a combination of techniques (XPS and EPR) [3]. Consequently, the phenol removal increased from 48% to 73% (under UV irradiation for 3 h), and from 7% to 15%, (under visible light for 3 h), with the most active ZnO nanorods surpassing the activity of commercial P25 TiO2 (Fig. c). The ZnO nanorods also proved to be a versatile photocatalyst achieving a high removal degree for a variety of pollutants under UV radiation for 3 h: bisphenol A (68%), rhodamine B (67%), and the pesticide imidacloprid (72%). Besides often showing enhanced activity, nanostructured photocatalysts also have limitations as they tend to agglomerate and are difficult to recycle. To overcome these limitations, we combined the prepared ZnO with polyacrylonitrile (PAN) fibers using electrospinning and freeze-drying. The obtained aerogel fibers were then shaped into a cylindrical mold (Fig. d). The obtained shaped photocatalysts were then utilized for continuous pollutant removal in a fixed-bed, continuous flow photoreactor.



References
[1] Nguyen, A. T. & Le Tran, L. Rev. Environ. Contam. Toxicol. 262, 11 (2024).

[2] Ong, C. B., Ng, L. Y. & Mohammad, A. W. Renew. Sustain. Energy Rev. vol. 81 536 – 551 (2018).

[3] Bai, S., Zhang, N., Gao, C. & Xiong, Y. Nano Energy 53, 296 – 336 (2018).

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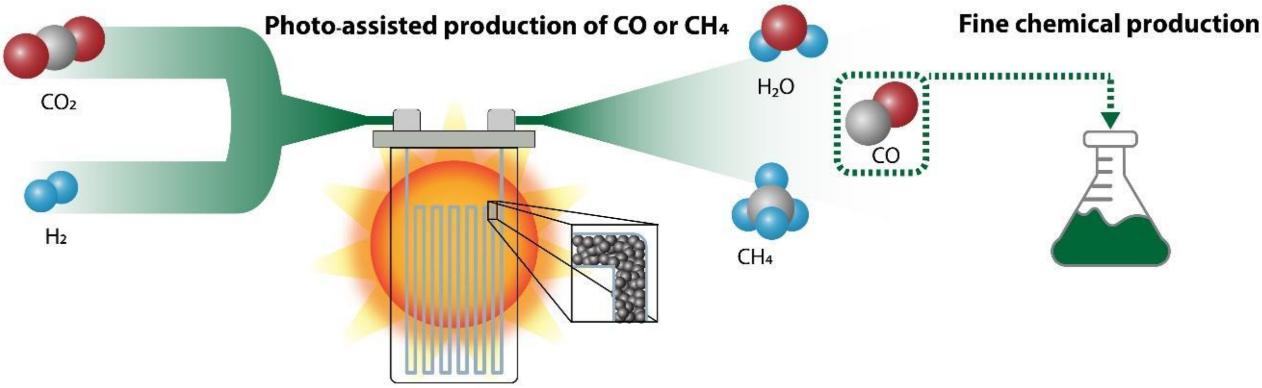
Title: **[OP55]** Light-assisted carbon dioxide reduction in an automated photoreactor system coupled to carbonylation chemistry

Abstract: Continuous-flow methodologies offer promising avenues for sustainable processing due to their precise process control, scalability, and efficient heat and mass transfer [1,2]. Because of their unique properties, flow reactors have found extensive applications, particularly in photochemistry, electrochemistry, and chemical systems that require strict temperature control. In the field of carbon dioxide reduction, a transition from the use of high temperatures and pressures in combination with non-sustainable energy in classical processes to alternative approaches is evident. One notable alternative is light-assisted carbon dioxide reduction, which exploits both thermal and non-thermal contributions to the processes. Continuous-flow reactors are particularly effective for these reactions and have been readily applied to carry out these transformations [3] .

To enhance the comparability of catalyst performance and establish guidelines for standardizing operational procedures, the advantages of continuous-flow have been applied to a novel reactor system [4]. This system emphasizes reproducibility, modularity, and automation, facilitating streamlined screening of conditions and catalysts. Through meticulous control over temperature, light intensity, pressure, residence time, and reagent stoichiometry, hydrogenation of carbon dioxide was conducted, yielding selective formation of carbon monoxide and methane using heterogeneous catalysts. Furthermore, the direct utilization of on-demand generated carbon monoxide in the production of fine chemicals via a carbonylative Suzuki coupling, aminocarbonylation, and alkoxycarbonylation was demonstrated. Tailoring the catalyst and operation conditions enabled stable carbon monoxide production required for these purposes.



References

[1] L. Buglioni, F. Raymenants, A. Slattery, S. D. A. Zondag, T. Noël, *Chem. Rev.* 2022, *122*, 2752–2906.

[2] J. H. A. Schuurmans, M. Peeters, M. Dorbec, K. P. L. Kuijpers, *J. Flow Chem.* 2024, *14*, 33–42.

[3] J. H. A. Schuurmans, T. M. Masson, S. D. A. Zondag, P. Buskens, T. Noël, *ChemSusChem* 2024, *17*, e202301405.

[4] J. H. A. Schuurmans, T. M. Masson, S. D. A. Zondag, S. Pilon, N. Bragato, M. Claros, T. den Hartog, F. Sastre, J. van den Ham, P. Buskens, G. Fiorani, T. Noël, *ChemRxiv.* 2024, DOI https://doi.org/10.26434/chemrxiv-2024-sz6ng.

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Title: **[OP56]** Pore Network Modeling of Hydrodynamics and Solute Dispersion in Packed Bed Reactors

Abstract: Packed Bed Reactors are widely used in various industries due to their effectiveness in facilitating chemical reactions. These reactors are filled with catalyst particles through which a fluid containing the reactants flows. The particle packing within the reactor provides a large surface area for reactions to occur and allows for the tailored residence time distribution of the reactants. However, this packing can also hinder fluid movement, leading to a significant pressure drop and potential flow maldistribution due to the packing configuration. Therefore, a detailed, locally-resolved understanding of the flow behavior inside such reactors is crucial for optimizing their design and performance.

In this study, we employed two approaches to investigate the hydrodynamics and solute dispersion in packed bed reactors: the Pore Network Model (PNM) as a meso-scale approach and Particle-Resolved Computational Fluid Dynamics (PR-CFD) as a micro-scale approach. The PNM simplifies the complex 3D porous geometry of the packed bed into a network of pores and throats, allowing for hydrodynamic and numerical simulations. This method provides local, partially-resolved results while being computationally efficient. In contrast, PR-CFD resolves the porous space into very fine grids, in this case 40 grid cells per particle diameter, and solves the Navier-Stokes and continuity equations on these grids. Although PR-CFD offers highly detailed, locally-resolved results, it demands significantly higher computational resources.

The number of computational elements in PNM is one or two orders of magnitude smaller than in PR-CFD, making PNM much faster and less computationally intensive. Despite its efficiency, and ability to capture average flow profiles, PNM does not capture all local pore-scale transport phenomena as effectively as PR-CFD.

In this study, we examined various geometric configurations with column-to-particle ratios of 4.2, 5.25, and 7 to evaluate how hydrodynamics, flow patterns, and mixing effects vary between these two simulation methods. Our findings indicate that PNM results are in good agreement with the PR-CFD results in the case of an almost homogeneous packing (N=7). Although PNM performs well at the average and pore levels, it fails to capture all local flow phenomena, leading to an underestimation of dispersion especially when the column-to-particle ratio is small.

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Title: **[OP57]** Hybrid water electrolysis: saving energy for the production of hydrogen

Abstract:

Improving the energy efficiency of the oxygen evolution reaction (OER), the anodic half-reaction in conventional water electrolysis, is one of the main challenges to address for the advancement of the electrochemical production of hydrogen at the industrial scale. Hybrid water electrolysis is an emerging field that makes use of an anode reaction alternative to the OER, usually the electrooxidation of small organic compounds, with the aim of reducing the overall energy requirements for the production of hydrogen. In this context, the electrocatalytic oxidation of low-cost alcohols is particularly attractive since they can be oxidized with lower energy costs compared to the OER using inexpensive transition metal oxide-based electrocatalysts in alkaline media.[1] Moreover, the partial oxidation of such alcohols can potentially lead to the formation of compounds of higher value than oxygen, increasing the economical attractiveness of the overall process. It is thus desirable to design electrocatalysts that are able to selectively convert low-cost alcohols into valuable products while simultaneously enabling high current densities, which are necessary for a high-rate production of hydrogen at the cathode.[1] In this presentation, the concept of “energy saving” of hybrid water electrolysis will be discussed. Examples will be provided, involving in particular $LaFe_{1x}Co_xO_3$ perovskites and Ni oxide nanoparticles as electrocatalysts for the electrooxidation of ethanol, isopropanol, and/or glycerol.[2, 3] This presentation will illustrate the usefulness of hybrid water electrolysis as an approach to save energy during the electrochemical production of hydrogen, as well as the current challenges that this emerging technology faces.

References

[1] F. van Lieshout, D. M. Morales, *ChemPlusChem* 2024, e202400182, in press.

[2] A. C. Brix, M. Dreyer, A. Koul, M. Krebs, A. Rabe, U. Hagemann, S. Varharde, C. Andronescu, M. Behrens, W. Schuhmann, D. M. Morales, *ChemElectroChem* 2022, 9, e202200092.

[3] D. M. Morales, D. Jambrec, M. A. Kazakova, M. Braun, N. Sikdar, A. Koul, A. C. Brix, S. Seisel, C. Andronescu, W. Schuhmann, *ACS Catal*. 2022, 12, 982–992.

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Title: **[OP58]** Evaluating the role of A-site deficiency and exsolution of Ni-Fe nanoparticles in Sr2-xFe1.5-yMo0.5NiyO6±δ electrocatalysts for co-electrolysis of H_2O and CO_2

Abstract: Perovskite oxides are a promising class of materials for use as fuel electrodes in solid oxide cell reactors. Among these, molybdenum-doped strontium ferrites(Sr_2-x$Fe_{1.5}$-y$Mo_{0.5}$Niy$O_6 \pm \delta$ x, SFMN) are particularly intriguing due to their high redox stability, electric conductivity and catalytic activity [1,2]. The performance of such perovskites can be further enhanced by the decoration of their surface with Ni-Fe exsolved under reducing environments, which act as catalytic active sites for electrolysis of H_2O and CO_2 for syngas production [3].

The number of metal nanoparticles that can be exsolved from the host oxide (i.e. SFMN) is determined by the amount of oxygen it can release during reduction. In order to stimulate exsolution, the oxygen reducibility of host oxide can be enhanced by introducing an A-site deficiency, which concurrently allows for the creation of a higher number of charge carriers within the structure and thus increases the conductivity.

Here, we developed various non- and A-site deficient SFMN fuel electrodes and we evaluate their performance in co-electrolysis environments. The developed electrodes are characterized by XPS, XRD, Rietveld Refinement and XRF to investigate the composition and structural properties of the as-prepared SFM and their exsolved counterparts. The exsolved Ni-Fe nanoparticles were characterized by XPS and SEM while the performance enhancement was evidenced through impedance spectroscopy and IV polarization. The present study demonstrates the potential of Ni-doped SFM fuel electrodes in enhancing the activity for co-electrolysis of H_2O and CO_2 in comparison to the state-of-the-art fuel electrode.

References

[1] S. Hou and K. Xie, “Enhancing the performance of high-temperature H_2O/CO_2 co-electrolysis process on the solid oxide $Sr_2Fe_{1.6}Mo_{0.5}O_{6-\delta}$-SDC/LSGM/Sr 2 $Fe_{1.5}Mo_{0.5}O_{6-\delta}$ -SDC cell,” Electrochim Acta, vol. 301, pp. 63–68, Apr. 2019, doi:10.1016/j.electacta.2019.01.164.

[2] Q. Liu, X. Dong, G. Xiao, F. Zhao, and F. Chen, “A novel electrode material for symmetrical SOFCs,” Advanced Materials, vol. 22, no. 48, pp. 5478–5482, Dec. 2010, doi: 10.1002/adma.201001044.

[3] D. Neagu, G. Tsekouras, D. N. Miller, H. Ménard, and J. T. S. Irvine, “In situ growth of nanoparticles through control of non-stoichiometry,” Nat Chem, vol. 5, no. 11, pp. 916–923, Nov. 2013, doi: 10.1038/nchem.1773.

[4] A. Mineshige et al., “Introduction of A-site deficiency into $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ and its effect on structure and conductivity,” Solid State Ion, vol. 176, no.11–12, pp.1145–1149, Mar. 2005, doi: 10.1016/j.ssi.2004.11.021.

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Title: **[OP59]** Modification of perovskite oxide-based electrodes for efficient H_2 production in Protonic Ceramic Electrolyzers

Abstract: Hydrogen production from water splitting in protonic ceramic cell reactors (PCCRs) is considered a promising approach for clean and renewable energy storage and transport at intermediate temperature (400-600 ° C) [1]. In such PCECs, steam is splitted (oxygen evolution reaction-OER) over the anodic electrode (positrode) while the protons created are subsequently transferred through the ceramic electrolyte to the cathodic electrode (negatrode) in order to produce H2. It is obvious that this system exhibits significant challenges regarding the choice of the electrocatalysts' components at anodic electrode to meet the sluggish reaction kinetics for OER and improve the electrochemical activity of PCCRs [2]. Herein, we have synthesized promising triple conducting (protons, oxygen ions, and electrons) perovskite oxides ($Pr_{0.95}Ca_{0.05}Ni_{0.5}Co_{0.5}O_{3-\delta}$, Ca-PNC) for H_2O electrolysis. Ca-PNC based-PCCR demonstrated a current density of 2.38 A cm^{-2} at 1.4 V and 650° C, three times that of the undoping PNC cell (0.79 A cm^{-2}) in electrolysis cell mode. Furthermore, the faradaic efficiency of the Ca-PNC cell exceeded 80% at 500° C, which is higher that PNC cell (~50%). DC four-probe and Electron paramagnetic resonance (EPR) techniques show that doping earth-alkaline Ca^{2+} in the A-site of $PrNi_{0.5}Co_{0.5}O_{3-\delta}$ (PNC) can not keep conductivity comparable to undoping-PNC, but also a higher oxygen vacancy concentration over un-doping PNC. More oxygen vacancies facilitate the water uptake of materials and reaction kinetics for OER, thereby an electrochemical activity for Ca-PNC based-PCECs. This finding provides insight into developing highly efficient oxide electrode catalysts for green hydrogen production IN PCCRs.

References

[1] E. Vøllestad, R. Strandbakke, M. Tarach, D. Catalán-Martínez, M.-L. Fontaine, D. Beeaff, D. R. Clark, J. M. Serra, T. Norby, "Mixed proton and electron conducting double perovskite anodes for stable and efficient tubular proton ceramic electrolysers," Nature Materials 2019, 18, 752-759, doi:10.1038/s41563-019-0388-2.

[2] F. Liu, H. Deng, D. Diercks, P. Kumar, M. Jabbar, C. Gumeci, Y. Furuya, N. Dale, T. Oku, M. Usuda, P. kazempoor, L. Fang, D. Chen, B. Liu, C.Duan, "Lowing the operatingtemperature of protonic ceramic electrochemcial cells to <450°C, " Nature energy 2023, 8, 1145-1157, doi: https://doi.org/10.1038/s41560-023-01350-4.

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Title: **[OP60]** Integration of in-situ water purification into zero-gap flow cell design for direct seawater electrolysis

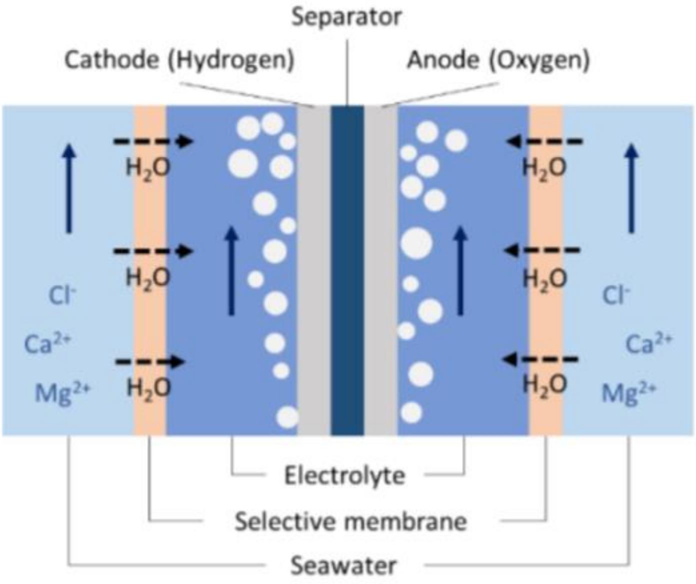
Abstract: In order to leverage the availability of offshore renewable energy and saline water, direct seawater electrolysis has become an interesting development for green hydrogen production. However, the challenge of seawater electrolysis lies in the presence of undesired ions in seawater, including Cl^-, Ca^{2+}, and Mg^{2+}, that facilitate degradation of the electrode. In addition, chloride oxidation reaction competing with oxygen revolution reduces Faradaic efficiency and bring safety concerns.

Commercial water electrolysis often relies on the reverse osmosis and ion exchange units to pretreat the water. To avoid these energy-intensive steps, there are several ways to make use the natural properties of the electrolyte and save the energy for water pretreatment. Selective membranes, including forward osmosis (FO) membranes and PTFE membranes, have been used for in-situ water purification [1][2]. Due to the difference of osmotic pressure or water vapor pressure across the membrane, the water is naturally drawn from the seawater to the electrolyzer unit without ions passing through the membrane (Figure 1). Such in-situ water purification makes energy-intensive pretreatment obsolete, while still avoiding contaminants to reach the electrodes.

In this project, we assess the potential for in-situ water purification in seawater electrolysis, and evaluate the stability and energy efficiency of such systems.

We integrate in-situ water purification into a zero-gap water electrolyzer flow cell and measure a critical component with weight-change measurements: the water transport rate across the FO membrane and the PTFE membrane, and calculated the corresponding limits in current density for steady state operation. Additionally, the selectivity of the membranes is investigated with ion chromatography. Finally, the in-situ water purification integrated into a zero-gap electrolysis flow cell is studied over 40hr. The degradation of the electrodes and the membrane is examined with electrochemical analysis and materials analysis (SEM/EDS).

The preliminary results show that the zero-gap flow cell integrated with FO membrane experienced pH-swing between anolyte and catholyte. Sodium ions, present in the electrolyte, becomes the dominant charge carrier and supresses the migration of protons across the proton exchange membrane. The acidity build-up leads to severe corrosion on the anode and generates new catalyst deposition on the cathode. The degradation mechanism shows that the limitation of using FO membrane in near neutral pH condition creates a fundamental constraint for the process. The PTFE-based membrane, however, can maintain a clean electrolyte without pH swing, and we provide directions for stable seawater electrolysis with in-situ purification.



References

[1] Veroneau, Samuel S., et al. *ACS Applied Energy Materials* **2022**, 5(2), 1403-1408.

[2] Xie, Heping, et al. *Nature* **2022**, 612(7941), 673-678.

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Title: **[OP61]** Towards Improving Negative CO_2 Emission: Optimizing Direct Air Capture Performance

Abstract: To achieve the Paris Agreement's 1.5°C target, it is essential to reduce carbon dioxide emissions to net zero and beyond by removing CO_2 from the atmosphere. Direct Air Capture (DAC) is a key technology in carbon dioxide removal, providing safe, flexible, and scalable negative emissions. The DAC process involves using a solid sorbent to extract CO_2 directly from the air. The sorbent is then regenerated using changes in temperature, pressure, or humidity, releasing CO_2 in a concentrated form for storage or conversion into valuable materials, such as chemical precursors. Unlike other negative emission strategies such as afforestation or bioenergy with carbon capture and storage, DAC is noted for its compactness and flexibility, enabling efficient integration with renewable energy sources and technologies. Enhancing and scaling up DAC is vital for reaching the net-zero carbon emissions goal by 2050. Current scientific efforts in DAC are primarily focused on developing sorbents and refining processes under specific laboratory conditions and experimental settings. It is crucial to recognize that DAC operations are extremely sensitive to variations in temperature and humidity, which can lead to capture costs to increase by up to 100% under adverse conditions. The expenses associated with DAC are closely linked to its energy requirements, necessitating the use of renewable energy sources like solar and wind, which are naturally variable. Hence, there is an essential need for the creation of a dynamic control and optimization mechanism to improve cost efficiency per tonne of CO_2 captured, a solution that remains unaddressed in existing research. To bridge this gap, we suggest utilizing advanced physics-based modelling, model reduction, and control system techniques. Our research proposes to model and optimize DAC systems under varying atmospheric conditions and intermittent power supply. We develop a high-fidelity model for the dynamic process of DAC to perform numerical experiments evaluating DAC operations under these fluctuating conditions and validating our methodologies. Subsequently, we analyze and manage the sensitivity of the system and process to the mentioned changes. Our research pioneers the development of strategies to optimize DAC efficiency and economic performance in real-world conditions, reducing costs and aiding in the large-scale adoption of DAC technology.

References

[1] Sabine Fuss and William F. Lamb et al. "Negative emissions—Part 2: Costs, potentials and side effects," Environmental research letters, vol. 6, no. 13, pp. 2016-2050, 2018.
[2] Ahmed Sodiq and Yasser Abdullatif et al. "A review on progress made in dac of CO_2," Environmental Technology & Innovation, vol. 29, p. 102991, 2023.
[3] Jan F. Wiegner and Alexa Grimm et al. "Optimal design and operation of solid sorbent direct air capture processes at varying ambient conditions," Industrial & Engineering Chemistry Research, vol. 61, no. 34, pp. 12649-12667, 2022.

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Title: **[OP62]** Investigation of droplets captured by filter materials at the mesoscale in oil-gas separators

Abstract: Understanding the intricacies of droplet behavior within this re-separation phase is vital, as it directly influences the efficiency and effectiveness of the oil-gas separator. The re-separation part is particularly challenging due to the small size of the droplets involved, necessitating sophisticated techniques to ensure their effective removal. By leveraging advanced computational tools combining Python and Blender, we can create detailed structures that replicate the random fiber arrangements in a mesoscale filter material of actual separators. Simulations with these structures allow us to observe and analyze how micro- and nano-droplets interact with the fibers, including their interception by the fibers, diffuse through the fiber matrix, and the effect of inertia on their trajectories. This approach will provide deeper insights into the mechanisms at play, enabling us to fine-tune the design of the fiber materials to enhance their separation capabilities.

A steady-state solver for the gas flow was coupled with a Lagrangian particle tracking solver for the droplets in OpenFOAM to investigate the collection of droplets mixed in the gas flow within mesoscale filter material structures. The Lagrangian solver incorporated the Cunningham correction factor for the Stokes drag force and the Brownian motion forces to accurately simulate (sub-)micron droplet behavior. The mesoscale filter material structures with fiber diameters between 3 and 5 μm and porosities between 0.925 and 0.975 were created and used to simulate gas flow and droplet collection.

The simulation results revealed that reducing the porosity and fiber diameter increases the pressure drop over the filter, but improves the droplet collection efficiency by increasing the surface area for droplet adhesion. The droplet collection efficiency and pressure drop were calculated and compared using analytical and empirical models taken from literature. This comparison validated the simulations and provided insights for optimizing fiber filter designs to improve filtration performance. The results of this study contribute to the development of more efficient microfiber media for applications requiring high filtration efficiency and low-pressure drop.

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Title: **[OP63]** Mass Transfer under Liquid-Liquid Slug Flow with Pickering Particles in Microreactors

Abstract: Microreactor technology has attracted considerable interest as an effective approach for enhancing existing chemical processes and discovering new reaction pathways. Researches into gas-liquid, liquid-liquid, and gas-liquid-liquid flow operations in microreactors has advanced significantly in chemical synthesis and purification. However, processes involving solid particles are still in their early stages due to the challenges of fouling and clogging in microchannels. Several strategies have been introduced to address the use of solid catalysts in biphasic reactions. One such approach involves slurry microreactors, where microparticles are suspended in the liquid phase to enhance heterogeneous catalysis. However, this method often results in limited particle utilization efficiency. In this regard, Pickering particles with dual wettability emerge as a promising solution since they can be irreversibly stabilized at the liquid-liquid interface to facilitate biphasic catalytic systems [1]. Herein, fundamental knowledge of mass transfer involving Pickering particles in microreactors is essential for a comprehensive understanding and optimization of the process performance.

In this work, both physical extraction (of ethyl acetate into water) and reactive extraction (of acetic acid into alkaline solutions) have been studied as model systems under slug flow processing in capillary microreactors made of polytetrafluoroethylene. Bare silica particles were chemically modified to possess different contact angles. The obtained hydrophilic particles were predominantly dissolved in the aqueous phase and hydrophobic particles in the organic phase. For physical extraction, slugs and droplets formed in the microreactor were separated at the outlet using a phase splitter based on their wettability difference. Then, the outlet concentration of ethyl acetate in the aqueous phase was analyzed with a UV–vis spectrometer, based on which the droplet-side mass transfer coefficient (k_L) could be calculated. For reactive extraction, a trace amount of phenol red was added as a pH indicator to the aqueous phase for flow visualization. By following the color change along the microchannel, k_L could be calculated according to the time at which the entire droplet turned from red to yellow (i.e., upon the completion of neutralization reaction).

From the experiments, the measured variation of slug and droplet lengths was analyzed, which allows the estimation of interfacial area (a) for mass transfer. Then, the influence of sodium hydroxide concentration, contact angle and loading of silica on droplet-side mass transfer was discussed. It was found that in the extraction of ethyl acetate, both the contact angles and solid loading did not show an obvious influence on mass transfer. However, when particles were immersed within droplets, a higher solid loading could result in a decline in the mass transfer coefficient. These findings can be further explained by the recirculation patterns and the behavior of various particles and solutes at the liquid-liquid interface.

References

[1] Chang F Q, Vis C M, Ciptonugroho W, et al. Green Chemistry 2021, 23 (7): 2575-2594.

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Title: **[OP64]** Dry fractionation of cohesive chickpea flour: impact of de-oiling and flow aids

Abstract: The transition from animal-based protein to sustainable plant-based protein is a major challenge in the food system. Processes to produce plant protein isolates consume water, chemicals and drying energy, and they are associated with a substantial environmental impact. Alternatively, protein-enriched ingredients, or protein concentrates, can be produced via dry milling and dry fractionation methods that do not involve energy-intensive drying steps.

Air classification is an industrially available approach to dryly concentrate protein from flours of starch-rich pulses such as peas and faba beans. However, the separation efficiency of chickpea flour is low compared to the other starch-rich pulses. This is attributed to chickpea flour being cohesive due to its comparably higher oil content and smaller starch granule size, which results in (liquid) oil bridging, increased Van Der Waals attraction and lower dry fractionation potential.

This research aimed to improve the properties of chickpea flour for dry fractionation via de-oiling and by blending in different types and concentrations of silica particles. Standardized air classification concentrated protein to a content of approximately 45%, which is similar to industrial practice. Initial protein yields below 25% could be increased to 70% by de-oiling, and this ingredient could be even further purified via electrostatic separation. Tested silica types doubled the initial protein yields, with lower concentrations being feasible for silica types consisting of nanosized primary particles. SEM(-EDS) image analysis revealed that higher concentrations increased the accumulation of nanoparticles onto flour particles, which lowered the basic flow energy of the flour and moderately increased its dispersibility in air. However, this did not yield additional protein upon air classification, hence silica blending did not seem to facilitate further microstructural disentanglement. Silica addition during impact milling produced similar but highly reproducible yields and omits blending.

Overall, protein yields benefited from de-oiling via additional microstructural breakdown and from flow aids via reduced fouling in the air classifier. The findings may contribute to improved fractionation and valorization of cohesive flours in general.

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Title: **[OP65]** Learning from Neural Networks: A Strategy to Identify Systematic Improvements to Activity Coefficient Models

Abstract: Following widespread adoption of activity coefficient models in routine process design tasks, deep neural networks (DNNs) offer a next-generation approach to the prediction of phase equilibria. Existing work demonstrates that their performance is on-par, if not better, than that of state-of-the-art thermodynamic models,[1] albeit single-purpose (e.g., only predicting the infinite dilution coefficient). On the one hand, activity coefficient models can be improved by incorporating more detailed descriptions of reality. On the other hand, identifying sources of systematic error requires careful study, deep understanding of the underlying inaccuracies and potential solutions. Traditional activity coefficient models derived from physics can often be used to calculate a multitude of related properties (e.g., excess enthalpy), and can therefore guide fundamental understanding in ways that many neural models currently cannot.

We posit that a hybrid approach—one where a DNN corrects a traditional activity coefficient model—may offer distinct synergistic advantages. It should improve the overall accuracy through closer representation of experimental data and subsequently that of related properties. Most interesting, however, is the potential to study the model's corrections to guide the identification of systematic improvements to the activity coefficient model.

In our work, we trained a DNN to not just correct the output of an activity coefficient model, but to adjust its central equations. After all, that is how new relations may be incorporated. This presents several challenges. Firstly, training neural nets requires outputs to be differentiable with respect to the net's parameters. They need to have a well-defined gradient. Or in other words: to allow a DNN to learn these types of corrections, the activity coefficient model itself, and any (non-linear) solver, needs to be differentiable. That is not a given. Secondly, neural networks are only as accurate as the data they are trained on. Yet, freely available, unlicensed thermodynamic data are rather scarce.

We offer a generalizable approach to learn corrections to undifferentiable activity coefficient models and show that we can markedly improve their performance. We then analyze the resulting corrections to search for new relations. Lastly, we identify potential gaps in available training data that could provide opportunities for further improvements.

References

[1] Medina, E. I. S., Linke, S., Stoll, M. & Sundmacher, K. Graph neural networks for the prediction of infinite dilution activity coefficients. *Digital Discovery* **1**, 216–225 (2022).

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Title: **[PP01]** Accurate 2D & 3D Simulations of Eddy Currents for Targeted Heating via Induction Heating

Abstract:

Induction heating has the potential to intensify many electrically powered chemical processes, including many endothermic reaction systems. Induction heating uses eddy currents and local resistance to produce Joule heating in the location of eddy currents. Control of local resistance and eddy currents can lead to rapid, localized heating. However, one must be able to predict the magnitude and location of heat produced, as well as the energy efficiency, to assess the potential of induction heating and to design an optimal workpiece.

In this work, an open-source eddy current solver built on the Open FOAM framework is utilized to simulate the eddy currents loops, and therefore the induction heating, for various optimized workpiece geometries. This model is adapted from previous work and is based on the A-Φ method for Maxwell's equations. Quantitative validation is achieved by comparing the numerical solution with the skin depth, and qualitative validation is attempted by comparing the results with thermal images from another study.

Serval novel geometries with significant process applications are presented. Notably, it is shown that control over the working resistance and eddy currents produced by induction heating can lead to increased homogeneity of temperature profiles in simulated reactors. By analyzing various geometries, it is shown how heat production can be distributed radially in the reactor, allowing for a more uniform temperature profile and efficient heating. This offers a promising pathway to not only use renewable energy, but also intensify various chemical processes by allowing for larger reactors than is currently viable.

This work provides a first starting point in the geometrical optimization of workpieces for inductively heated chemical reactors.

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Title: **[PP02]** Modelling framework for Direct Air Capture process: Investigating CO_2-H_2O co-adsorption on amine functionalized sorbents

Abstract: The increasing concentration of atmospheric CO_2 necessitates the development of effective direct air capture (DAC) technologies. The study presents a comprehensive modelling framework for the adsorption process in DAC, focusing on the mathematical and numerical modelling across three distinct scales: particle, reactor, and process. Attention is put in understanding CO_2-H_2O co-adsorption phenomena. At the particle scale, a detailed particle model is developed to facilitate kinetic analysis and coupled with the reactor model providing insights into the adsorption kinetics and thermodynamics, essential for optimizing and assessing the direct air capture performance. Co-adsorption kinetics is currently investigated using TGA analysis. At the reactor scale, various configurations, including packed bed, monolith, and fluidized bed reactors, are modelled to understand the influence of reactor design on CO_2 capture efficiency. These models incorporate fluid dynamics and heat transfer mechanisms, offering a predictive tool for reactor design and operation optimization. At the process scale, a Temperature Vacuum Swing Adsorption (TVSA) model is being developed to optimize the overall DAC process. The TVSA model integrates the particle model and reactor models to evaluate different operational strategies, aiming to maximize CO_2 capture while minimizing energy consumption and operational costs.

The multi-scale modelling approach provides a holistic understanding of the DAC process, identifying key parameters and operational conditions that influence performance. The findings highlight the critical role of reactor design and operational strategy in enhancing the efficiency and scalability of DAC technologies.

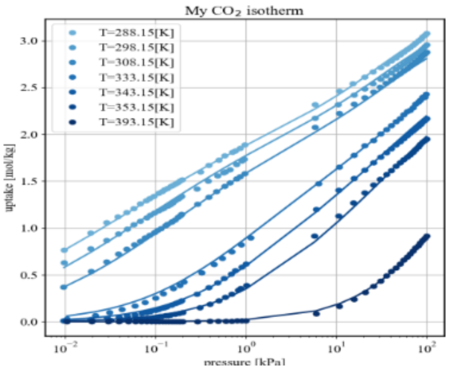

Fig. 1. Dry CO_2 isotherm fitting with Toth-Langmuir model.

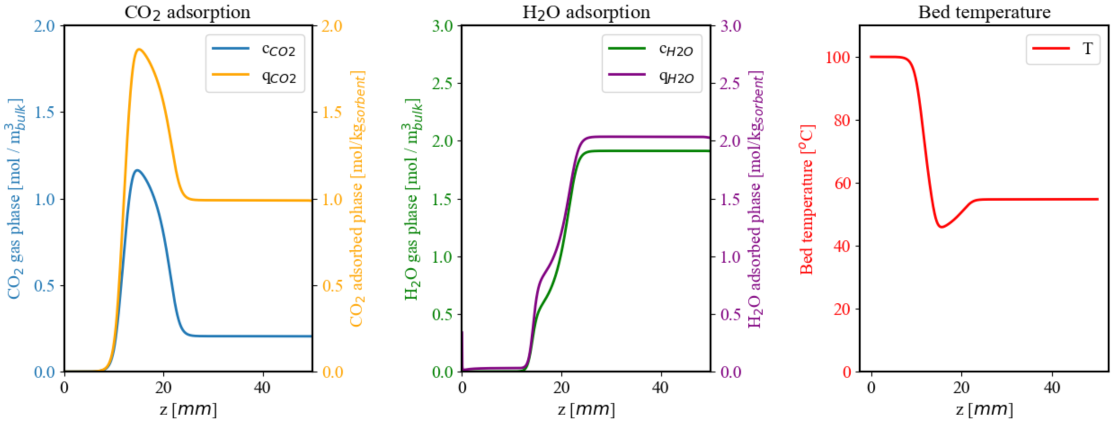

Figure 2. Axial packed bed profiles during CO_2 and H_2O adsorption.

References

[1] May-Yin Ashlyn Low et al., J. Of Chemical & Engineering data 68 (12), 3499-3511.

[2] Young, John and García-Díez et al., Energy Environ. Sci., 2021

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Title: **[PP03]** Selectivity control between Reverse Water-Gas Shift and Fischer-Tropsch Synthesis in Carbon-supported Iron-based Catalysts for CO_2 Hydrogenation

Abstract: CO_2 hydrogenation to chemicals and fuels has the potential to alleviate CO_2 emissions and displace fossil resources simultaneously via consecutive RWGS and FTS reactions, also known as CO_2-FTS. As Fe-based catalysts are active and selective for both reactions, their bifunctionality requires a delicate balance between the RWGS and FTS. In this work, we investigated the thermodynamic constraints of RWGS and CO_2-FTS, the influence of CO_2 conversion on selectivity and the influence of Fe nanoparticle size within the range of 4.7 to 10.3 nm. An inert carbon support was selected to rule out metal-support interaction and promoting effects of the support. Catalytic performance was evaluated at 300 °C, 11bar, $H_2/CO_2/Ar = 3/1/1$, 600 to 72000 $mL \cdot gcat^{-1} \cdot h^{-1}$. At a CO_2 conversion level below RWGS equilibrium conversion of 23%, RWGS was found to be the primary and dominant reaction. No primary Sabatier reaction was observed. At higher CO_2 conversion till the CO_2-FTS threshold of 42%, the secondary FTS reaction became dominant. Notably, a positive non-linear relation between CO_2 conversion and CO selectivity was discovered. Comparing two catalysts with identical 5 wt. % Fe loading but different average Fe nanoparticle size (6.6 and 8.4 nm), the 8.4 nm Fe catalyst was at least two times more active than the 6.6 nm Fe catalyst. In situ Mössbauer spectroscopy suggested a positive correlation between particle size, carburization and selectivity towards long-chain hydrocarbons. For these potassium-promoted carbon-supported Fe-based catalysts, nanoparticles of at least 8 nm are required for the formation of Fe carbides and improved reactivity.

References

[1] A. Saravanan, et al. A comprehensive review on different approaches for CO_2 utilization and conversion pathways, Chem. Eng. Sci. 236 (2021) 116515.
[2] W. Zhou, et al. New horizon in C1 chemistry: breaking the selectivity limitation in transformation of syngas and hydrogenation of CO_2 into hydrocarbon chemicals and fuels, Chem. Soc. Rev. 48 (2019) 3193-3228.
[3] S. Lyu, et al. Stabilization of ε-iron carbide as high-temperature catalyst under realistic Fischer-Tropsch synthesis conditions. Nat. Commun. 11 (2020) 6219.
[4] P. Wang, et al. Synthesis of stable and low-CO_2 selective ε-iron carbide Fischer-Tropsch catalysts. Sci. Adv. 4 (2018) eaau2947.

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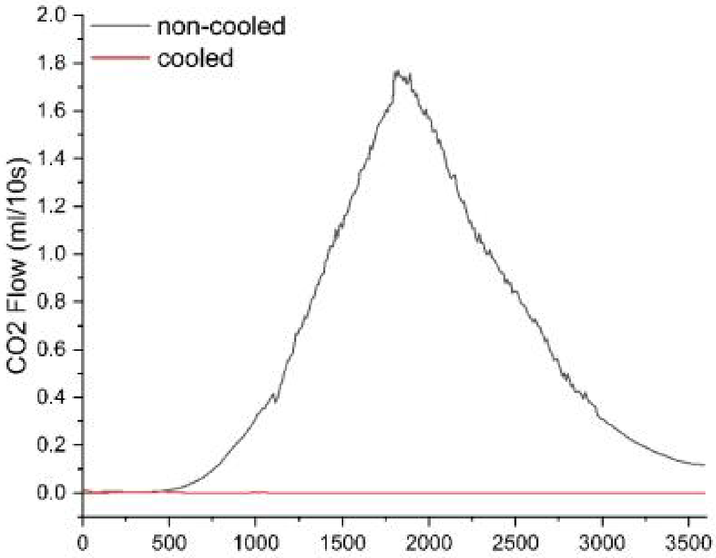
Title: **[PP04]** Syngas Production by Plasma-Assisted Decomposition of $KHCO_3$ in an Integrated Carbon Capture and Utilization Process

Abstract: Adsorption of CO_2 from flue gasses or air using solid materials is a method to effectively reduce ambient CO_2 concentrations. Conventionally, modulation of temperature or pressure is performed to desorb captured CO_2 and regenerate the sorbent. The obtained CO2 can be then stored or converted into value-added products in a separate process. Plasma can be used to desorb CO_2 as well. Due to the energetic nature of plasma, CO_2 is chemically activated and converted into, for example, CO during the desorption. This opens up the possibility of combining CO_2 capture and CO_2 utilization in one single process[1].

Plasma enables highly endothermic reactions such as the decomposition of CO_2 into CO and O_2. Previously, artificial photosynthesis which convert CO_2 and H_2O into syngas simultaneously, has been investigated[2]. Potassium carbonate is a sorbent material that adsorbs CO_2 and H_2O in a one-to-one ratio at ambient conditions. This opens up the possibility of using potassium bicarbonate for integrated CO_2 capture and utilization using a wet CO_2 stream. During the desorption H_2 and CO are formed. This work explores the plasma- assisted decomposition of $KHCO_3$ into CO_2 and H_2O and the in-situ production of syngas from the decomposition products.

It was found that $KHCO_3$ is not directly decomposed by plasma because no CO_2 or H_2O formation was observed during plasma exposure. However, Due to Joule heating by the plasma, the reactor reached a sufficient temperature to allow for thermal $KHCO_3$ decomposition. H_2, CO, and O_2 were found among the reaction products, confirming the possibility of in-situ syngas production. At higher plasma powers, the H_2 over CO ratio increased, due to a reduced CO_2 conversion. At high H_2O concentrations, that are reached at high plasma powers because of faster $KHCO_3$ decomposition, the CO_2 conversion is reported to reduce because of the back reaction of CO with HO to CO_2 and atomic hydrogen[2] . Both the plasma power and the dilution of carrier gas during the plasma-assisted decomposition of $KHCO_3$ can be used to tune the H_2/CO ratio.



CO_2 flow for a cooled and a non-cooled plasma reactor

References

[1] Li S, Ongis M, Manzolini G, Gallucci F, Non-thermal plasma-assisted capture can conversion of CO_2 , Chemical Engineering Journal (2021).

[2] Ma X, Li S, Ronda-Lloret M, Chaudhary R, Lin L, Van Rooij G, Gallucci F, Rothenberg G, Raveendran S, Hessel V, Plasma Assisted Catalytic Conversion of CO 2 and H 2 O Over Ni/Al_2 O_3 in a DBD Reactor, Plasma Chemistry and Plasma Processing (2019).

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Title: **[PP05]** Investigating deactivation and kinetics of levulinic acid hydrogenation on titania supported ruthenium catalysts

Abstract: Among a multitude of chemicals that can be obtained from lignocellulosic biomass, γ-valerolactone (GVL), produced via levulinic acid (LA) hydrogenation, can be used as a solvent and fuel additive. The hydrogenation of LA typically takes place under aqueous phase conditions.1 Recent trends on Ru-catalyzed LA hydrogenation have led to a variety of catalytic supports being used. Amongst these, TiO_2 has shown promising catalytic activity albeit suffering from deactivation. This work utilizes typical industrial conditions (T>100°C) to investigate stability and LA hydrogenation kinetics upon deactivation (i.e., stabilization of activity). Ru/TiO_2 was synthesized via incipient wetness impregnation techniques using $RuCl_3$ as the precursor. Catalytic activity testing was performed in a packed bed reactor with upflow conditions.

The deactivation rate decreases with temperature. This is in stark contrast with sintering as the main cause of deactivation, favoured at high operating temperatures and higher water partial pressures. Specific surface area of active metal particles reduced over time resulting in drop of catalytic activity. Additionally, an increase in Ru^0 content with longer time on stream suggests in-situ reduction and change in the catalytic structure with reaction time. Besides, no ruthenium was detected with ICP analysis of the liquid reaction sample; and no significant differences in the TGA curves of spent catalysts from different time-on-streams.

To determine the effect of Ru loadings on deactivation kinetics, active metal loading was increased and later, total catalyst mass was increased while maintaining similar Ru loading on the support. Both the catalytic beds showed significantly slower deactivation kinetics compared with 100 mg 1wt% Ru/TiO_2. LA conversion after achieving stabilization of catalytic activity increased five-fold after its initial deactivation. Further studies using the stabilized catalytic bed revealed a zero and half-order reaction kinetics with respect to LA and hydrogen, respectively.

This work shows that the deactivation rate of titania-supported ruthenium catalysts is slower at higher temperatures. Sintering and changes in the ruthenium oxidation state are the primary causes for deactivation in aqueous phase LA hydrogenation. We report a first-order dependence on LA for the aqueous phase hydrogenation kinetics. This is applicable for catalysts stabilized after initial deactivation and not at the beginning of the catalyst lifespan. Decoupling the rate of sintering and changing ruthenium oxidation state might be beneficial in optimizing reaction and catalytic parameters for LA hydrogenation.

References

[1] ACS Catal. 2014, 4, 4, 1171–1181.

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Title: **[PP06]** Methanol synthesis from CO_2 using a co-precipitated ZnO/ZrO_2 catalyst in a continuous spinning basket reactor

Abstract: Methanol is one of the key building-block-chemicals that has been utilized in various sectors of human life for the past decades [1]. Until now, it is mainly produced from fossil-based syngas as its feedstock [2]. This condition leads as a strong driver to shift toward a more sustainable process by using renewable carbon sources such as CO_2. A potentially appealing route to produce methanol involves CO_2 hydrogenation using renewable H_2 [3]. However, catalyst development for industrial methanol synthesis utilizing CO_2 is still in the infant stage [4]. Recently, studies have indicated the convincing performance of ZnO/ZrO_2 catalyst for methanol synthesis from CO_2, in terms of conversion and product selectivity [5]. We here report the performance of a co-precipitated ZnO/ZrO_2 catalyst (13% mol Zn) to synthesize methanol from CO_2, as a renewable carbon feedstock, in a continuous spinning basket reactor. The reactor setup is connected to an online GC-FID through a traced line for exit gas composition analysis. Two gas feeds with approximately the same CO_2:H_2 ratio (1:3) were used, one containing only CO_2, and the other one containing a mixture of CO and CO_2 as the carbon sources. The reactions were performed under relatively mild conditions at a temperature range of 200-300°C, a constant pressure of 20 bar, a stirring speed of 1000 rpm, and a space velocity of 11 $m^3 .kg^{-1} .h^{-1}$. We observed the increasing value of the important performance indicator, namely methanol space-time yield and CO_2 conversion, as the temperature rose to 300°C. The highest methanol space-time yields were 1.16 and 1.25 (mmol methanol. g^{-1} cat. h^{-1}) respectively, for CO_2 -only feed and a mixture of CO and CO_2 along with the CO_2 conversion reaching up to 6%. This result may be beneficial for the advancement of catalyst development and process technology in renewable CO_2 conversion to methanol and beyond.

References

[1] Beck, A., Newton, M. A., van de Water, L. G., & van Bokhoven, J. A. (2024). Chemical Reviews, 124(8), 4543-4678.
[2] Sollai, S., Porcu, A., Tola, V., Ferrara, F., & Pettinau, A. (2023). Journal of CO_2 Utilization, 68, 102345.
[3] del Pozo, C. A., Cloete, S., & Álvaro, Á. J. (2022). Energy Conversion and Management, 266, 115785.
[4] Wang, J., Li, G., Li, Z., Tang, C., Feng, Z., An, H., ... & Li, C. (2017). Science advances, 3(10), e1701290.
[5] Sha, F., Tang, S., Tang, C., Feng, Z., Wang, J., & Li, C. (2023). Chinese Journal of Catalysis, 45, 162-173.

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Title: **[PP07]** Investing energy in hydrogen – accelerating applications of decentralised hydrogen

Abstract: The Professional Doctorate project deals with the complex challenges and strategic goals related to energy, sustainability, and circularity, focusing on the transition towards green energy and the role of hydrogen in addressing these challenges. The "Energy & Sustainability" domain outlines six missions, including achieving climate neutrality in raw materials, products, and processes, and reaching 80% circularity by 2050 (source: UAS-PD program guideline, 2022; KIA Climate and Energy, 2019). A key aspect of the energy transition is the generation and distribution of green energy, influenced by location and timing of energy production relative to demand. Increased electrification has led to grid congestion due to mismatches between electricity generation and consumption, while natural gas use has decreased due to geopolitical factors and increasing prices.

To address these challenges, the Dutch industry is exploring hydrogen as a solution for energy storage and transportation. Hydrogen can help balance supply and demand, easing grid congestion, and can be transported via existing natural gas infrastructure, which is being adapted into a hydrogen backbone across the Netherlands by 2030 (source: GasUnie, TenneT, 2021). However, a major barrier to progress is the current mismatch between the supply of green hydrogen and the unclear demand from industry, slowing the energy transition (source: inaugural lecture R.L. van Leeuwen, 2022).

The PD project focuses on two regional industrial use-cases along the hydrogen value chain: biofermentation at Twence and water purification at the Waterschap Vechtstromen. These use-cases aim to make the processes more sustainable by exploring how residual flows can be reused and how CO_2 emissions can be minimized or valorized. For example, biofermentation converts organic waste into biogas but also emits CO_2, posing a challenge in finding ways to capture and use these emissions for producing C-based chemicals. In water purification, the project investigates the potential of using treated effluent instead of drinking water for hydrogen production, promoting circularity in water use. It also addresses energy efficiency in water treatment plants, emphasizing the need to reuse energy and materials.

Beyond technical challenges, non-technical factors like labor market shortages and a lack of specialized training are also major obstacles. The project emphasizes the importance of developing new skills and expertise, aligning educational programs with industry needs, and fostering learning communities around hydrogen (source: Human Capital Roadmap 2020 – 2023).

Overall, the PD project aims to advance regional sustainability efforts, develop techno-economic models for industrial processes, and create authentic learning environments to support the workforce transition towards green hydrogen and circular economy practices.

References

[1] “GasUnie, TenneT, 2021. HyWay 27: waterstoftransport via het bestaande gasnetwerk?”, https://www.rijksoverheid.nl/documenten/rapporten/2021/06/30/eindrapport-onderzoeksproject-hyway27

[2] “Topsectoren, 2019. KIA Energietransitie & Duurzaamheid.” , https://www.topsectoren.nl/publicaties/publicaties/2019-publicaties/oktober/161019/kia-energietransitie-en-duurzaamheid

[3] “Topsectoren, 2020-2023. Samen aan de slag, roadmap Human Capital.”, accessed 26 June 2024, https://www.topsectoren.nl/publicaties/kamerstukken/2019/november/12-11-19/roadmap-hc-topsectoren.

[4] UAS-PD program guideline, 2022. Professional Doctorate Energy & Sustainability.

[5] “van Leeuwen, R., 2022. Nieuw Evenwicht: Naar een duurzaam energiesysteem”, https://www.saxion.nl/onderzoek/areas-and-living/duurzame-energievoorziening

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Title: **[PP08]** The Utilization of Humin Ozonolysis Product via Bioconversion using Oleaginous Yeast

Abstract: The humin formation as a byproduct in thermochemical conversion of sugars, or sugar-containing feedstock like biomass, is unavoidable. It reduces the main product yield and causes intensive reactor maintenance, among other issues. Several attempts have been made to optimize the main conversion process and maximize the humin utilization [1]. Humin depolymerization by ozonation is one method that can be applied in mild operating conditions. The ozonolysis reaction produces an oil composed of shorter components in the form of carboxylic acids and esters if using alcohols as solvent. This humin-derived oil needs to be further upgraded to maximize its value. Bioconversion of the oil by using oleaginous yeasts to produce single-cell oil is a promising application. Yeast are known to be able to utilize several forms of carbon as feedstock, including hydrocarbons, lipids and derivatives, and short carboxylic acids, and some of them can transform these molecules into lipids under suitable conditions [2].

The humin-derived oil obtained in this study is mainly composed of carboxylic acids, i.e., oxalic acid, malonic acid, and succinic acid. Around 1.5 % w/w of humin-derived oil in demineralized water was applied as the sole carbon source for the yeast Yarrowia lipolytica MUCL 28849. After 72 h, the cells were harvested and processed to extract the intracellular lipids. The results showed that the lipid yield in the presence of the oil was at 13.76 % w/w, slightly higher than the cell control at 13.23 % w/w. The lipid extract was derivatized to methyl esters and analyzed by GC-MS to identify its composition. The fatty acids composition of lipid from the treatment with the carbon source was similar to the cell control containing oleic, linoleic, palmitic, palmitoleic, and stearic acid with the amount of 32.4, 30, 14.8, 9.4, and 4.2 % respectively. On the other hand, the broth was analyzed via GC-MS (after ester derivatization), HPLC, and NMR analyses. The GC-MS results indicated the consumption of two components in the oil i.e. oxalic acid and succinic acid, because the corresponding retention time at 2.79 and 7.05 min respectively were no longer available compared to the carbon source control and feedstock chromatogram. These results were supported by HPLC analysis where the peak of oxalic acid became less intense. The C-NMR results confirmed the previous analysis that the chemical shifts profile in the range of 50-55, and 165-175 ppm corresponding to alkyl and carboxylic groups respectively were changed. This proof concept study showed that *Yarrowia lipolytica* MUCL 28849 was able to utilize the humin oil as the carbon source and produce lipids out of it.

References

[1] S. Liu et al., Appl. Energy Combust. Sci., vol. 10, 2022, doi: 10.1016/j.jaecs.2022.100062.
[2] Gao et al. Biotechnol Biofuels., vol. 13:3, 2020, doi: 10.1186/s13068-019-1645-y.

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Title: **[PP09]** Pyrolytic Decomposition of Methane to Hydrogen and Functional Solid Carbon: Multi-Scale Modeling and Reactor Development

Abstract: The increasing global demand for sustainable energy and functional materials requires the development of new technologies for large-scale production of energy carriers and materials. One of these technologies that have gotten more attention recently is the catalytic pyrolysis of methane. During the pyrolysis, methane is decomposed into hydrogen gas and carbon nanomaterial, without direct greenhouse gas emissions. The carbon accumulates on the catalyst particles, causing growth of the irregular angular particles during reaction, as well as deactivation of the catalyst [1].

The growth of the particles (as much as 70 g_c/g_{cat}) causes a particle size distribution (PSD) in the reactor. In a fluidized bed reactor, this polydispersity will cause a change in fluidization behavior as well as potential segregation caused by partial defluidization [2]. In a continuous system, fresh small catalyst particles would be fed to the reactor, while larger spent catalyst particles are continuously removed. Due to the complexity of the system, little is known on the impact of catalyst growth on the reactor performance and hydrodynamics.

In this work, a combined experimental and modelling approach is used to quantify the effects of the irregularly shaped particles and the PSD present in the reactor. Experiments are conducted using spent methane pyrolysis catalyst particles of different sizes in a pseudo 2D fluidized bed using PIV-DIA to measure the fluidization behavior [3]. Monodisperse samples are used to measure the pressure drop and minimum fluidization velocities of the different sized particles, which are compared to equations found in literature to enable more accurate modelling of the system [4]. Polydisperse samples are used to study the potential for segregation based on particle sizes within the reactor.

A CFD-DEM model is developed to predict the fluidization behavior of both the monodisperse system, taking into account the irregular and angular shape, and the polydisperse system, showing the segregation behavior seen in the experiments. The experimental data was used to validate the model. The CFD-DEM model enables numerical studies on the hydrodynamic effects caused by the PSD, and enables predicting the fluidization behavior and reactor performance of a polydisperse fluidized bed with irregular particles.

References

[1] M. Hadian et al., ‘Kinetic study of thermocatalytic decomposition of methane over nickel supported catalyst in a fluidized bed reactor’, Chem Eng Sci.

[2] O. O. Olaofe et al., ‘Particle Mixing and Segregation in Gas-Solid Fluidized Beds Containing Binary Mixtures’, ECI Symposium Series.

[3] M. J. V. Goldschmidt et al., ‘Digital image analysis measurements of bed expansion and segregation dynamics in dense gas-fluidised beds’, Powder Technol.

[4] D. Kunii et al., ‘Fluidization and Mapping of Regimes’, Fluidization Engineering.

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Title: **[PP10]** Taking off with Furfural: The missing link in the production of high performance jet fuel

Abstract: To challenge climate change and decrease societies reliance on fossil recourses, we need to develop new routes for producing fuels and chemicals. This especially holds for aviation, which is recognized as a challenging sector to electrify or convert to H_2, and will rely on hydrocarbon fuels for decades to come.

Besides several certified routes to produce SAF by the ASTM[1], we report here on another route based on Furfural, a promising platform chemical that can be derived from lignocellulosic biomass.[2-3]

Many different routes for the upgrading of furfural to fuels are known.[2-3] The most important steps consist of C-C coupling followed by deep hydrogenation. A promising pathway that also delivers very desirable cycloalkanes is to upgrade furfural to cyclopentanone and couple it with more furfural via aldol condensation, a route solely based on biomass derived furfural.[4] Cycloalkanes indeed delivers the high energy density that is desired for blend-in jet fuel.

The industrial scale implementation of furfural derived bio jet is however, still in its infancy. Challenges arise in the synthesis of the required cyclopentanone from furfural, as significant heavy side products are produced leading to CPO yields of 50 mol%. [5] However, research has shown that control over key parameters such as concentration and pH, can lead to control over molecular weight distribution, yielding Gasoline, Diesel and Vacuum Gas Oil (VGO) fraction, eligible for valorized by thermal and/or catalytic cracking.[6]

In our endeavor to achieve the large scale production of furfural-derived jet fuels, our focus has been on formulating a comprehensive process design. However, we have encountered significant challenges arising from the varied demands of each reaction involved. To tackle these complexities, our efforts have been directed towards extensive investigations encompassing the reductive rearrangement of furfural into cyclopentanone, subsequent aldol condensation reactions involving furfural and cyclopentanone, and the subsequent deep hydrogenation process along with requisite separation steps. Our primary aim remains the development of a unified and operationally efficient integrated process design.

References

[1] K. Siew, Renewable and Sustainable Energy Reviews, 2021, 150, 111502
[2] J.-P. Lange, ChemSusChem. 2012, 5, 150-166
[3] J.-P. Lange, Catalysis Today Volume 435, 1 June 2024, 114726
[4] L. Ao, RSC Adv., 2019, 9, 3661
[5] R. Baldenhofer, ChemSusChem, 2024
[6] J. Buijtenen, WO2011076736, 2011

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Title: **[PP11]** Combined catalytic dehydrochlorination and pyrolysis for PVC waste stream

Abstract: PVC is primarily used for building materials: flooring, windows, cables, pipes and coatings. In addition, due to its flexibility, PVC is used for medical purposes such as blood bags.

All these performances are possible due to the incorporation of a wide range of additives. These additives enhance the thermal and mechanical properties of PVC products and significantly expanding the applications. PVC products are known for having a long service life compared to other plastics materials, although they will end up as solid waste [2] and will require a proper disposal. One of the possible options is the recycle/upcycle of the PVC. Today PVC end-of-life products are recycled mainly by mechanical recycling, but new technologies for chemical recycling are under development.

The chemical (feedstock) recycling is more suitable for unsorted plastic mixtures and waste streams containing composite materials. This research is specifically centered on this topic; starting from pure PVC and pure PVC waste and expanding the knowledge to mixed stream containing PVC and chlorinated materials. Upcycling processes will be studied to obtain secondary valuable feedstocks through thermal treatments, such as (catalytic) pyrolysis.

Before pyrolysis, an additional step is needed to partially remove chlorine (dehydrochlorination step), posing specific challenges, including damage to common materials due to the corrosive properties of the resulting gases, mostly composed by HCl.

The kinetic control of the dehydrochlorination process is fundamental, as well to avoid the formation of dioxins [3], and can be achieved using heterogeneous catalysts to lower temperature.

References

[1] Plastic Europe. (2021). Plastics the Facts.

[2] Mehdi Sadat-Shojai, Gholam-Reza Bakhshandeh. (2011). Polymer Degradation and Stability, 4, 404. DOI:10.1016/j.polymdegradstab.2010.12.001.

[3] Krzysztof Lewandowski, Katarzyna Skórczewska. (2022). Polymers, 15, 3035. DOI: 10.3390/polym14153035

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Title: **[PP12]** Coupling Mild Flow-through Organosolv Extraction and Catalytic Oxidation from Lignocellulosic Biomass with High S-type Units towards Benzoquinones

Abstract: Effective lignin valorization towards specific aromatic chemicals is a pivotal step in the economically feasible biorefining process. As the most abundant aromatic biopolymer, lignin with high amounts of syringyl units utilized to yield elevated monomeric contents being particularly striking. The current lignin valorization methods exhibited some intractable challenges such as harsh conditions, low degradation efficiency and undesired target products. Herein, this study reports an integrated conversion strategy involved in mild organosolv fractionation in a flow-through setup and lignin oxidative depolymerization to facilitate the selective production of aromatic benzoquinones. The alcohol-incorporated lignins from different biomass with high S-type units can be oxidized into 2,6-dimethoxy-1,4-benzoquinone (DMBQ, max 18% yield) under relatively mild reaction conditions (100 °C, air). The yields of target monomers are different based on different lignin linkages and aromatic units from different lignocellulosic feedstocks. It is noteworthy that in the mechanism of exploration, phenolic moieties in lignin model compounds are very crucial in lignin oxidation, which also be influenced by the different functional groups in side chain of aromatic rings. This work provides the mechanism insight and potential in the successive procedure for mild lignin-to- chemicals valorisation.

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Title: **[PP13]** Modelling Aromatization in a Fluidized Bed Reactor

Abstract: Green and plastic waste can be recollected and via pyrolysis converted to gaseous hydrocarbons, with carbon numbers up to C50. In order to increase the product value of waste recycling, the gas, after pyrolysis, can be further processed. The further processing of the gas is performed in a Fluidized Bed Reactor filled with zeolite catalyst to convert the hydrocarbons towards aromatics, mostly benzene, toluene and xylene (BTX). These aromatics are valuable base chemicals that are currently obtained with fossil fuels. The pyrolysis of plastic waste provides an alternative using renewable resources.

A working demo plant is in place at the Dutch company BioBTX. But in order to go to industrial production scale, more insight is needed into the reaction kinetics. Additionally, to allow for optimization of the design of the industrial scale FBR, validated models are required.

A Computational Fluid Dynamics model is coupled with the Discrete Element Method (CFD-DEM). The catalyst particles are modelled via Newton’s laws of motion, while the continuum (gaseous) phase is described by the local averaged Navier-Stokes equations. This model is used to provide insight into the influence of different process parameters on the fluidization behavior.

A phenomenological model is currently being designed to increase the computational efficiency of modelling results. Computational efficiency often comes at the expense of modelling accuracy, it is important that the right assumptions are drawn from the CFD-DEM model and experiments. If the phenomenological model is validated, this model can be used to perform a parameter study to optimize the design of the industrial scale FBR.

Additionally, this model will be designed such that the implementation of all the physical phenomena such as; the reaction kinetics, convection, mass and heat transfer. By a modular implementation of especially the reaction kinetics, it is possible to change the reaction kinetics to a different case and use this model to describe other fluidized bed reactors.

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Title: **[PP14]** 1D model of droplet drying using interface receding approach

Abstract: Spray dryers are widely used in different industries, e.g. food, chemical and pharmaceutical industries. One of the most important phenomena in spray drying process is the drying of droplets. The drying of droplets containing dissolved or suspended solids consists of four stages: heat-up, constant rate drying (shrinkage), falling rate drying (solidification), and final dry particle heating [1]. Traditional numerical approaches include the characteristic drying rate curve [2] and the reaction engineering approach (REA) [3]. However, these methods are semi-empirical with the necessity of knowing the critical moisture content or activation energy, respectively. In addition, these methods do not account for the spatial distribution of temperature and moisture within the droplet.

In this study, the drying of a single droplet containing suspended solids is simulated with an interface receding approach based on a simultaneous heat and mass transfer [4]. In this model, heat is transferred convectively from the surrounding air to the droplet's surface in the constant rate period, causing free water to evaporate and the droplet's outer radius to decrease. During the falling rate period, a receding evaporation interface separates the wet core from the dry crust, which moves to the center of the droplet as water evaporates from the wet core. The increasing heat and mass transfer resistances result in a decreasing evaporation rate. This period ends when the existent water in the wet core is fully evaporated.

For the constant rate drying, a variable grid size algorithm is applied due to the shrinkage, while the grid size is fixed in the falling rate period because the droplet size remains constant. All equations are solved implicitly with Tridiagonal Matrix Algorithm (TDMA) and discretization scheme is applied based on the physics of the phenomenon (using central, backward, and forward discretization).

The model successfully predicts the droplet's temperature, water vapor concentration, and mass loss profiles, when comparing to experimental results of Nesic and Vodnik [1]. Moreover, the model is able to predict the internal temperature and concentration distribution.

References

[1] Nešić, S., & Vodnik, J. (1991). Chemical EngineeringScience, 46(2), 527-537.
[2] Langrish, T. A. G., & Kockel, T. K. (2001). T Chemical engineering journal, 84(1), 69-74.
[3] Chen, X. D., & Xie, G. Z. (1997). Food and Bioproducts Processing, 75(4), 213-222.
[4] Dalmaz, N., Ozbelge, H. O., Eraslan, A. N., & Uludag, Y. (2007). Drying Technology, 25(2), 391-400.

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Title: **[PP15]** Aramazing – Chemical Recycling of Aramid Materials

Abstract: Plastic materials have become indispensable for the entire humanity with usages in almost every industry, including car tires or clothing. Given the demands in sustainability, it is desired to change the current situation of plastic disposal, which is generally sent to landfill and incinerated after use.

The project at hand focuses on establishing a design for an upscaled aramid recycling pilot plant. Aramids (Twaron®) are plastic fibres of huge importance for the production of various technical products, such as personal protective equipment, ballistic vests, or car tires, with superior properties such as heat resistance and high tensile strength [1]. To reduce the ecological footprint, Teijin Aramid plans to depolymerize end-of-life para-aramid fibres (poly para- phenyleneterephthalamide – PPTA) into their building blocks: p-phenylenediamine (PPD) and terephthalic acid (TA). This would transform the aramid production process into a circular one. Mechanical and physical techniques are being used as well to recycle aramids. However, not all aramid recycle feedstock is of the right quality for these routes, either being too contaminated or too degraded. Thus, there is a need for chemical recycling.

PPTA is depolymerized using a hydrothermal liquefaction (HTL) technology. Based on the empirical information obtained after performing laboratory scale experiments, it is desired to conduct the modelling of the entire pilot plant in a flowsheeting tool.

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References

[1] Institute of Sustainable Process Technology, 2023. Aramazing: Sustainable Aramids. URL https://ispt.eu/projects/aramazing/ (accessed 15 May 2024)

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Title: **[PP16]** Cooperative integration of thermal solar and wind energy with molten salts and green ammonia enables sustainable power generation in Morocco

Abstract: Providing electricity in a sustainable and affordable manner is key to curve down the greenhouse gas emissions. In the African continent this is a paramount challenge due to the harsh environmental conditions, limited access to power distribution networks, and complex geopolitics. This calls for innovative solutions for robust power generation. To address this issue, we have studied the combination of concentrated thermal solar towers and wind turbines to satisfy fluctuating daily energy demand at a cost competitive levelized cost of electricity (LCE) in Morocco due to the high solar radiation and wind energy availability in this location. Molten salt energy storage (MSES) was used to compensate daily fluctuations in demand and supply, while green ammonia was used as energy storage vector for seasonal fluctuations. A model was developed to find optimal storage capacity for MSES, Wind farm size, power to ammonia to power (P2A2P), and concentrated solar power (CSP) plant sizes to realize the minimal LCE. Favorable results were obtained in which LCE's of combined CSP-wind systems are lower at 0.098 $/kWh than for systems in which wind and solar do not cooperate at 0.20 $/kWh and 0.104 $/kWh respectively. Additionally, MSES was found to be a requirement for satisfying daily demands while ammonia storage was found to have minimal contribution to lowering LCE. Surprisingly, the minimum LCE was obtained using a hybrid system of 58% CSP generation capacity and 42% wind generation with a 10 kg NH3/h Ammonia production capacity and a MSES capacity of 13 hours for a 140 MW peak demand grid. This is due to the complementary wind and solar energy generation profiles over the year in the region of Oued ed Dahad-Lagouira in Morocco. These results highlight the importance of combining complementary energy sources and storage systems to achieve the most competitive solutions for sustainable electricity generation.

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Title: **[PP17]** Process simulation of stepwise pyrolysis of cashew nut shell via Aspen Plus

Abstract: The production of cashew nuts results in cashew nutshell (CNS) waste, necessitating effective valorization strategies. This study investigated a stepwise pyrolysis approach, driven by the diverse properties of pyrolysis products and their distinct applications. In the first step, CNS is heated at low temperatures (<200°C) to extract cashew nutshell liquid (CNSL), rich in valuable components, for example, cardanol, cardol and anacardic acid, which has applications in pharmaceutical, oil and gas industries, adhesives, and surfactants [1] . The second step is raising the temperature to around 500°C to carbonize the remaining CNS waste, producing biochar for use as fuel, soil amendment, and in emerging applications for biocarbon-based composite materials.

This work simulated the stepwise pyrolysis of CNS process in Aspen Plus® with a feed capacity of 6000 tons per year. A steady-state model using chemical kinetics was developed to predict pyrolysis product yields under various reactor conditions and feedstock compositions.

The simulation model was validated by comparing the product distribution, gas, liquid, and char composition with experimental and literature data, at temperatures 400, 500, and 600 °C [2, 3]. The model was then used to analyze the CNS properties (moisture content, the residual proportion of CNSL) and pyrolysis process conditions (pyrolysis temperature: 200-700°C; residence time: 1-360 seconds) on product yields and power generation. Optimal conditions for maximizing pyrolysis oil and char yields (38% and 24% respectively, with 38% gas) are identified at 500°C with a 180-second residence time. Energy balance analysis indicates that combustion of non-condensable gases can sustain the entire process at 500°C with sufficient surplus energy for miniature electric power generation. The heating values of the bio-oil and biochar are 30.2 MJ/kg and 28.6 MJ/kg respectively, indicating their potential as high-energy fuels.

This simulation model can serve as a robust tool for CNS pyrolysis optimization, product utilization, and techno-economic analysis of the CNS stepwise pyrolysis plant. This will enable further refinement of the process design, optimizing both economic and environmental outcomes.

References

[1] Kyei, S.K., et al., A comprehensive review on waste valorization of cashew nutshell liquid: Sustainable development and industrial applications. Cleaner Waste Systems, 2023: p.100116.

[2] Ábrego, J., et al., Pyrolysis of cashew nutshells: Characterization of products and energy balance. Energy, 2018.158: p.72-80.

[3] Kaur, R., et al., Characterization of slow pyrolysis products from three different cashew wastes. Bioresource Technology, 2023. 376: p. 128859.

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Title: **[PP18]** Techno-economic analysis of circular plastic production using induction heating

Abstract: The global rise in plastic production, driven by population growth and changing lifestyles, is contributing to a significant increase in greenhouse gas emissions, with predictions indicating a rise from 4.5% in 2015 to 18% by 2050 (1). To mitigate this, a shift from fossil-based to circular plastics is essential. Pyrolysis, is emerging as a promising technology for converting mixed plastic waste into high-quality feedstock for new plastic production. Induction heating at the laboratory scale has demonstrated up to 80% energy savings compared to traditional heating methods (2).

This study focuses on a techno-economic analysis of scaling-up a plastic pyrolysis process powered by induction heating. An Aspen Plus simulation model of the pyrolysis reactor has been created, where 100 kg/h of waste high-density polyethylene (HDPE) are processed into 11.7 kg/h of oil product and 88.3 kg/h of gas product at 550°C. The study also considers different separation train options targeting alternative products such as Liquefied Petroleum Gas (LPG) via a cryogenic separation and CO_2 by implementing a Pressure Swing Absorption (PSA) process for CO_2 capture after the combustion of the gas product stream.

The analysis will then assess the implications of scaling up, focusing on how the reactor design (such as reactor type, operating mode, residence time, etc.) is affected by this heating technology. Furthermore, the study will evaluate the impact of the various separation train configurations and the associated costs to determine their influence on the overall feasibility of the process.

The expected outcomes include identifying key factors that significantly impact the final cost, providing recommendations for process optimization, and understanding the potential impact of induction heating on process design and economics compared to alternative heating technologies. This analysis will offer valuable insights into the adoption of induction heating in plastic pyrolysis, contributing to the development of more economically viable recycling technologies. The findings will help in understanding how to effectively transition from fossil-based to circular plastics, reducing the environmental footprint of the plastic industry.

References

[1] Stegmann P, Daioglou V, Londo M, van Vuuren DP, Junginger M. Plastic futures and their CO_2 emissions. Nature.2022 Dec;612(7939):272–6.

[2] Wong SL, Armenise S, Nyakuma BB, Bogush A, Towers S, Lee CH, et al. Plastic pyrolysis over HZSM-5 zeolite and fluid catalytic cracking catalyst under ultra-fast heating. J Anal Appl Pyrolysis.2023 Jan 1;169:105793.

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Title: **[PP19]** A Closed Carbon Cycle Approach for Full Valorization of Lignocellulosic Biomass

Abstract: This research addresses the global priority of improving resource efficiency, aligning with the United Nations Sustainable Development Goal 12.2 for sustainable management and efficient use of natural resources by 2030 [1,2]. The study explores the development of a novel integrated approach for the complete valorization of lignocellulosic biomass fractions based on a method for the efficient extraction of high-quality lignin.

The research employs a closed-loop, semi-continuous flow system using ethanol as a green solvent for extraction. This innovative process recovers and reuses ethanol, which is also produced as a by-product and reintroduced into the system, creating a sustainable carbon cycle.

The extraction of lignin from biomass using this flow-through system has demonstrated remarkable results, achieving up to 90% delignification efficiency [3]. Key findings include high-quality lignin extraction with high β-O-4 conservation, crucial for its valorization into aromatics via hydrogenolysis.

A key challenge for such organosolv extractions with alcohols is the formation of a complex hemicellulose derived sugar fractions. Novel analytical methods (HPLC, NMR) have been developed to identify, characterize, and quantify these products, addressing a significant challenge in the field. The research has successfully valorized alkyl sugars into furfural, a high- value chemical, with over 70% yield.

The study also demonstrates the potential for combining residual cellulose from the extraction process with alkyl sugars from lignin purification for enzymatic saccharification into monomeric glucose, achieving over 65% conversion efficiency. Ongoing research aims to optimize the conversion of monomeric glucose into bioethanol using S. cerevisiae, building upon established processes [4].

References
[1] C. Mair, R. Asada, in: 2019, pp. 1–11.
[2] UNECE, Sustainable Use of Natural Resources (n.d.).
[3] D.S. Zijlstra, J. de Korte, E.P.C. de Vries, L. Hameleers, E. Wilbers, E. Jurak, P.J. Deuss, Front Chem 9 (2021).
[4] S.A. Alrumman, Brazilian Journal of Microbiology 47 (2016) 110–119.

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Title: **[PP20]** Mitigating Hydrogen Crossover in Alkaline Water Electrolysis (AWE)

Abstract: Alkaline water electrolysis (AWE) has emerged as a highly efficient method for green H_2 production.[1] However, the integration of AWE with renewable energy encounters major challenges, since the inherent power fluctuations frequently result in low current densities. Under these conditions, H_2 crossover through the diaphragm can result in elevated hydrogen in oxygen (**HTO**) concentrations. Eventually, the H_2 crossover can result in an explosive mixture. Consequently, safe operation of AWE frequently requires preemptive shutdowns, thereby limiting the technology's flexibility.[2]

The main mechanism leading to such elevated HTO concentrations is considered to be diffusion.[3] Interestingly, introducing a finite cathode-diaphragm gap has been found to offer significant advantages over the industrial standard, which typically contain a zero-gap configuration.[2] Once dissolved H_2 now reaches the diaphragm, its concentration has decreased significantly due to the increased path length. The more gentle concentration gradient across the diaphragm then reduces H_2 diffusion to the anode.[4] In the current work, we aim to locate the optimal gap size, and investigate the effects of pressure, temperature, electrolyte flowrate and current density on the HTO concentration. These findings are used to extend the safe operating regime of AWE to lower current densities, thereby enhancing AWE's compatibility with renewable energy resources.

References

[1] Brauns, Jörn, and Thomas Turek. "Alkaline water electrolysis powered by renewable energy: A review." Processes 8.2 (2020): 248.
[2] de Groot, Matheus T., Joost Kraakman, and Rodrigo Lira Garcia Barros. "Optimal operating parameters for advanced alkaline water electrolysis." international journal of hydrogen energy 47.82 (2022): 34773-34783.
[3] Bernt, M., et al. "Analysis of gas permeation phenomena in a PEM water electrolyzer operated at high pressure and high current density." Journal of The Electrochemical Society 167.12 (2020): 124502.
[4] Barros, Rodrigo Lira Garcia, et al. "Impact of an electrode-diaphragm gap on diffusive hydrogen crossover in alkaline water electrolysis." International Journal of Hydrogen Energy 49 (2024): 886-896.

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Title: **[PP21]** Minimizing ohmic resistance in alkaline water electrolyzers

Abstract: Green hydrogen's prominence in the energy transition is undeniable, particularly as an energy carrier, storage solution, and chemical reagent. Among various production techniques, alkaline electrolysis stands out due to its reduced reliance on noble and rare earth metals and its advanced technology readiness level (TRL). However, high current density operation faces challenges due to ohmic resistance limitations. Despite a plethora of investigations into electrodes, diaphragms, and bubble dynamics, a consensus on the optimal configuration for industrial deployment remains elusive.

As part of this study, a holistic approach is undertaken to assess ohmic resistance with electrochemical impedance spectroscopy alongside I-V measurements[1]. Lab-scale flow cells have been tested with a variety of electrode substrates and diaphragms, while concurrently developing simple cell designs to ensure precise control of the gap distance between electrodes and diaphragm, along with exploring the potential incorporation of reference electrodes[2].

First tests on different diaphragms like Zirfon, Sample X (procured from a private vendor), and PES were conducted. Results reveal the PES separator to exhibit the lowest ohmic resistance (see figure 1). Furthermore, no significant increase in ohmic resistance with current density is observed for each test, indicating limited influence of bubbles in this zero gap cell configuration. Additionally, investigations on Ni perforated plates are conducted, with bubble behavior analyzed using a high-speed camera. Its expected that these findings pave the way for a substantial reduction in ohmic resistance, thereby realizing an efficient alkaline electrolyzer.

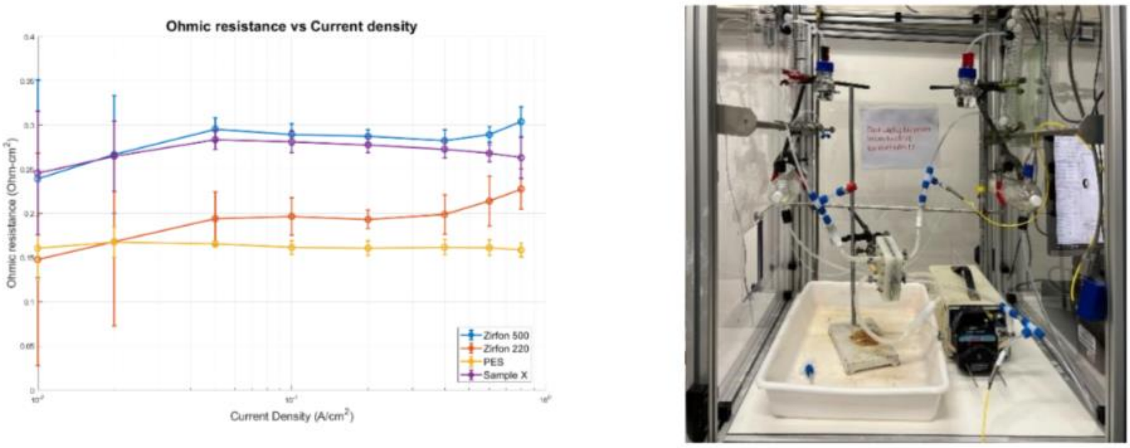

Figure1 Alkaline water electrolysis setup

References

[1] Rodríguez, J.; Palmas, S.; Sάnchez-Molina, M.; Amores, E.; Mais, L.; Campana, R. Simple and Precise Approach for Determination of Ohmic Contribution of Diaphragms in Alkaline Water Electrolysis. Membranes, 2019, 9, 129.https://doi.org/10.3390/membranes9100129

[2] Rodrigo Lira Garcia Barros, Joost T. Kraakman, Carlijn Sebregts, John van der Schaaf, Matheus T. de Groot. Impact of an electrode-diaphragm gap on diffusive hydrogen crossover in alkaline water electrolysis. International Journal of Hydrogen Energy, 2023. https://doi.org/10.1016/j.ijhydene.2023.09.280

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Title: **[PP22]** PyDOLPHYN: Dynamic modelling for optimal system integration of water electrolysis

Abstract: Improving operational flexibility of electrolysers is one the major challenges to ensure large-scale implementation of green hydrogen production. In particular, identifying the optimal operating strategies that allow to couple electrolysers with intermittent energy sources such as wind and solar, while ensuring safe and efficient operations, is still a challenging task. A recently developed Python-based dynamic simulator (PyDOLPHYN) will be introduced [1].

PyDOLPHYN uses a set of physics-based non-linear models to dynamically simulate and optimize multi-energy assets. This allows to bridge the gap between high-level energy system modeling tools and detailed process-level and multi-physics software. We report the results for two case studies related to green hydrogen production assets. First, we proved how multi-objective optimization based on dynamic simulations is crucial to avoid unfeasible or extremely expensive designs. Secondly, we studied how asset-level operational strategies impact the profit when the asset is connected to both electricity and hydrogen markets. We showed that by using a sufficiently complex logic (i.e., combining a MILP approach with the non-linear models) more profitable operations (+32%) can be identified.

References

[1] Javier Fatou Gómez, Alejandro Martín-Gil, Simone Dussi PyDOLPHYN: Dynamic simulations and optimization of multi-energy assets, manuscript under review (2024)

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Title: **[PP23]** Electrochemical flow modelling of a semi-solid flow battery

Abstract: Simulation results of the flow and electrochemical performance of an organic semi-solid redox flow battery (ssRFB) are presented. A multi-physics computational model was developed at the cell-level to understand the impact of different cell designs. First, a flow model able to capture the non-Newtonian behavior typical of a ssRFB was calibrated with rheological experimental data. Different cell designs have been then simulated in 3D to gain insights from the flow profile. Pitfalls of the base cell design was clearly revealed and included e.g. the presence of stagnant zones. Variations of this design have been then explored, ranging from adding a number of parallel paths inside the reaction zone to differently shaped flow distributors upstream. Insights on how these variations impact flow homogeneity and pressure drops will be discussed. Finally, a steady-state electrochemical model has been developed assuming one-way coupling with the flow behavior, i.e., the velocity profile influences the electrochemical part (species transport and reaction) but not vice versa. Different parameter sensitivities (on flow conditions and reaction parameters) are explored and their impact on the current-voltage curve of the battery are reported. The model will be compared with experimental data and in future projects will be used to guide the fabrication of a novel reactor design.

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Title: **[PP24]** Indirect CO_2 capture: extracting CO_2 from concentrated seawater using bipolar membrane electrodialysis

Abstract: To achieve net zero emissions by 2050, we need CO_2 as a resource for synthetic fuels and chemicals (e.g. long-distance transport) and negative CO_2 emissions to offset hard-to-abate emissions (stemming from e.g. agriculture). Hence, CO_2 capture from the environment will be indispensable. We present a method to indirectly capture CO_2 from the air via seawater using bipolar membrane electrodialysis (BPMED) induced pH swing. Bipolar membranes generate H^+ ions that convert seawater's dissolved inorganic carbon (DIC) to a gaseous stream of CO_2 while generated OH^- ions precipitate DIC in the form of $CaCO_3$.

First, we start by proposing and modelling (Aspen Plus) process flow diagrams that employ the BPMED unit and utilize two liquid streams: concentrated seawater (waste product of a reverse osmosis plant) and demineralized seawater (main product of the reverse osmosis plant) to produce CO_2 and $CaCO_3$ as gaseous and solid products, respectively. Second, we construct a lab-scale version of the preferred process and experimentally evaluate its performance, identifying the limiting factors, and commenting on the implications.

In our model, we compare *in-situ* and *ex-situ* BPMED processes. In the *in-situ* process, DIC conversion to CO_2 is initiated inside the BPMED unit while in the *ex-situ* process, DIC conversion to CO_2 and $CaCO_3$ happens downstream of the unit. We find that the *ex-situ* process shows lower energy consumption, which follows from the smaller amount of fluid to be processed in BPMED and thus reduced pumping power. Additionally, the *ex-situ* process limits the pure water consumption.

The experiments show strong deviations from the expected BPMED voltage when using concentrated seawater. We identify that the deviation originates from $Mg(OH)_2$ precipitation on the surface of cation-exchange membranes inside the BPMED unit. Removing all Mg^{2+} ions from the concentrated seawater allows us to maintain the expected BPMED voltage. The final BPMED energy consumption from concentrated seawater is 112 kJ mol^{-1} CO_2 (for Mg^{2+} free process) which is lower than previous work on CO_2 capture from seawater (155 [1] and 242 [2] kJ mol^{-1}, respectively).

References

[1] Digdaya, I. A.; Sullivan, I.; Lin, M.; Han, L.; Cheng, W.-H.; Atwater, H. A.; Xiang, C. Nature Communications 2020, 11 (1), 4412.

[2] Eisaman, M. D.; Parajuly, K.; Tuganov, A.; Eldershaw, C.; Chang, N.; Littau, K. A. Energy & Environmental Science 2012, 5 (6), 7346-7352

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Title: **[PP25]** Steady-state and dynamic modeling of a CO_2 electrolyzer: membrane electrode assembly

Abstract: The electrochemical reduction of CO_2 offers a promising route to low-carbon production of fuels and bulk chemicals when powered by renewable electricity. However, to satisfy the flexibility needs of renewable power systems, it is crucial to anticipate the capabilities and limitations of the electrolyzer for seamless operation during power ramps.

While integrating water electrolyzers with renewable energy sources has been investigated through several dynamic models, there is a lack of CO_2 electrolyzer models suitable for power system flexibility studies. In this project, we investigate the applicability of a semi-lumped model of a single electrolyzer cell to predict the performance of the electrolyzer subjected to load changes. We study the membrane electrode assembly configuration, as its high energy efficiency makes it an attractive design for industrial application. This dynamic model provides a fast screening of the transient responses of the electrolyzer to input potential changes. The model is validated at steady state conditions using the results of a high-spatial-resolution model from the literature.

The semi-lumped model helps to evaluate the effect of intermittent potential on current density, overpotentials, faradaic efficiency, CO_2 conversion and utilization in the cell. Additionally, such a model helps to investigate the transient response time for various input changes. This is particularly important from the viewpoint of system control and performance optimization, in order to increase the transient capabilities of the unit.

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Title: **[PP26]** Scalable fabrication of catalysts for proton exchange membrane water electrolysis

Abstract: The phenomenal growth in renewable power generation has even further increased research interest in the fields of energy storage and material conversion through electrolysis. A key element in any electrolysis process is a catalyst tailored to the targeted reaction, e.g., platinum group metals (PGMs) for water splitting. Due to the immense scale of the problem, and the cost and scarcity of PGMs, economical use of these materials is imperative. Hence, catalysts are typically dispersed on a support material, e.g., Pt-loaded carbon black (Pt/C) as cathode catalyst in proton exchange membrane water electrolysis (PEMWE). Compared to bulk Pt, a larger fraction of atoms is exposed at the surface thus leading to a higher catalytic activity per unit weight of Pt. Traditional fabrication methods for Pt/C, such as incipient wet impregnation, allow control over the amount of deposited Pt; however, the morphology and dispersion are very difficult to control with this method.

In this work, we propose an alternative and economically feasible fabrication route Pt/C catalyst layers based on gas-phase synthesis via atomic layer deposition (ALD). We have previously shown that Pt/C can be fabricated via atmospheric pressure ALD on particles in a fluidized bed (ALD-FBR), which is readily scalable [1]. In contrast to traditional fabrication methods, we can control the morphology and achieve a finer dispersion of deposited Pt [1,2], enabling higher catalytic activity at reduced Pt loading. First, we use ALD-FBR to fabricate tailored Pt/C for PEMWE. Second, to establish the relationship between morphology and performance, we characterize the material using (HR)TEM and with respect to electrochemically active surface area (ECSA) as a relative indicator for performance. However, a full assessment of Pt/C requires testing in real-world applications, which is why we go one step beyond bare catalyst characterization and demonstrate the use of ALD-made Pt/C in lab-scale PEMWE cathodes. In conclusion, we demonstrate, for the first time, the fabrication of Pt/C via atmospheric pressure FBR-ALD, and its superior performance at reduced Pt loadings compared to conventional Pt/C in PEMWE cathodes.

References

[1] F. Grillo, H. Van Bui, J. A. Moulijn, M. T. Kreutzer, and J. R. van Ommen, “Understanding and Controlling the Aggregative Growth of Platinum Nanoparticles in Atomic Layer Deposition: An Avenue to Size Selection,” J. Phys. Chem. Lett., vol. 8, no. 5, pp. 975–983, Mar. 2017, doi: 10.1021/acs.jpclett.6b02978.

[2] F. Grillo, J. A. Moulijn, M. T. Kreutzer, and J. R. van Ommen, “Nanoparticle sintering in atomic layer deposition of supported catalysts: Kinetic modeling of the size distribution,” Catal. Today, vol. 316, pp. 51–61, Oct. 2018, doi: 10.1016/j.cattod.2018.02.020.

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Title: **[PP27]** Gas holdup optimization in zero-gap alkaline water electrolysis via multiphase modelling

Abstract: Currently, the majority of the hydrogen is produced as fossil fuel based grey hydrogen. To decrease the dependency on fossil fuels, green hydrogen production is a promising replacement. This technology uses sustainable energy sources for water electrolysis without producing harmful side products. The generated hydrogen can be used as chemical as well as energy carrier. As energy carrier, water electrolysis copes with the problematic energy surplus created by sustainable energy sources in peak hours. However, the current water electrolysis technologies have low efficiencies and high costs. Therefore, this study strives to optimize the process, specifically the zero-gap alkaline water electrolysis (AWE) method where hydroxide is used as electrolyte.

The optimization focuses on reducing the gas holdup, a major factor influence on the efficiency. The gas holdup has a double negative impact on the system. Firstly, bubble nucleation on the electrode results in loss of active surface area. Secondly, the bubbly flow hinders the electrolyte flow, necessary to complete the electronic cycle. To limit the gas holdup, the 3D structure of the electrode is investigated. Furthermore, the potentials of applying a coating on the electrode is researched.

For this research a numerical model is being developed. The model is made in OpenFOAM and is based on the open-source OpenFuelCell2 toolbox, an Euler-Euler multiphase model. To convert the toolbox to an AWE simulation, user defined functions are implemented for the electrochemistry, gas-crossover and temperature. The inclusion of all three phenomena allow for an accurate description of the experimental setup, which is used for validation. In this study, the preliminary results will be presented on the implementation and efficiency improvement.

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Title: **[PP28]** Nanostructuring Ni-based porous transport layers for anion exchange membrane water electrolysis

Abstract: Electrochemical water splitting is a promising alternative for producing large-scale green hydrogen. Recently, Anion Exchange Membrane Water Electrolysis (AEMWE) is garnering special attention due to its advantages such as use of low-cost materials and higher efficiencies over conventional techniques such as Alkaline Water Electrolysis (AWE) or Proton Exchange Membrane Water Electrolysis (PEMWE).

In the development of anodic electrodes for AEMWE, nickel-based mixed-metal (oxy)hydroxides are considered as promising low-cost substitutes to expensive noble metal catalysts such as IrO_2 and RuO_2. Here, Ni-based porous transport layers (PTLs) which also act as the electrocatalysts are used as anodes in a membrane electrode assembly. Since in AEMWE, the PTL surface also serves as the active site, surface engineering provides further avenues to improve the performance of emerging AEMWE systems. Helium plasma irradiation is a potential technique that can fabricate self-supported nanostructures on these PTLs. The plasma irradiation technique has been extensively studied in relation to the surface erosion and embrittlement of fusion reactors [1,2]. Recently, a few studies have applied this technique for green hydrogen production [3-5]. Herein, we extend the application of this technique to fabricate nanostructured PTLs that can overcome the limitations of traditional catalyst layers containing ionomer and nanoparticle catalysts.

The results indicate that the MEA with the nanostructured PTL's delivers ~25% higher performance than its bare/unmodified counterpart, and the combination of mixed-metal (oxy)hydroxides surpass commercially available PTL/electrocatalysts. The current results provide a promising route for combining the versatile nature of plasma technology and the desirable characteristics of mixed-metal (oxy)hydroxides for fabricating next-generation water splitting devices. Going forward, influence of ionomers, durability and performance is expected to be correlated.

References

[1] 1. D. Dasgupta et al., *Nucl. Fusion*, 59, 086057 (2019).
[2] S. Kajita, A. M. Ito, and K. Ibano, *J. Appl. Phys.*, 132, 181101 (2022).
[3] S. Feng et al., *Appl. Surf. Sci.*, 580, 151979 (2022)
[4] Ranade et al., *Adv. Mater. Interfaces.* 10, 2300486 (2023)
[5] Ranade et al., *Appl. Surf. Sci.*, 669, 160413 (2024)

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Title: **[PP29]** Alkaline water electrolysis beyond 3 A/cm^2

Abstract: The production of green hydrogen is a pathway for balancing the intermittency of green energy production and for energy conversion, such as Power-to-X. Alkaline water electrolysis is the most mature technique for producing green hydrogen on scale, however, it is still struggling with technical challenges such as low operating current densities, high resistances, and low operating flexibility. We seek to address those issues by incorporating catalyst coated diaphragms (CCDs) into a zero-gap electrolyser, allowing us to significantly lower the potential via the minimization of ohmic resistances and reduction of cathodic and anodic overpotentials. CCDs are state of the art industrial diaphragms, where the catalyst is applied directly on top of the diaphragm, to improve the electrode – diaphragm interplay.

Alkaline water electrolysis using CCDs (Zirfon UTP 500 and UTP 220) was conducted at current densities from 0.002 up to 3.5 A/cm^2 at varying temperatures (20 – 75 °C) in 30 wt.% KOH. Using simple and platinum group free catalysts (Raney Ni; FeNi LDH) we reached 3.5 A/cm^2 at less than 2.3 and 2.5 V for Zirfon UTP 220 and 500, respectively. The improvements were linked mainly to a reduction in the kinetic overpotential due to better catalytic properties and an increase in active surface area. The CCDs were stable under room temperature for up to 60 h at a constant current density, however, showed degradation at 75 °C over the course of 240 h.

We further assessed the effect of increasing the concentration of electrolyte Fe on the performance of the CCDs. We could observe that an addition of Fe using an anodic catalyst with high Fe content, did not lead to drop in the overpotential. However, when the anodic catalyst was low in Fe content, we could observe an improvement with increasing electrolyte Fe concentration.

The CCDs were further assessed suing SEM/EDX to obtain information on the change in surface properties post electrolysis. We could observe that even in Fe rich electrolyte, leaching of Fe from the FeNi LDH was observed, which lead to the fracturing of the CCD and thus deactivation. On the Raney Ni we observed a deposition of Fe on the Raney Ni particles over extended periods of time, however, the surface structure stayed intact.

This research shows that it is kinetically realistic to design and operate a high performance alkaline water electrolyser at current densities beyond 2 A/cm^2.

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Title: **[PP30]** Atomic Layer Deposition for Proton-Exchange Membrane Water Electrolysis

Abstract: Proton-exchange membrane (PEM) water electrolysers represent the forefront of hydrogen production through water electrolysis. However, they heavily rely on platinum group catalysts and titanium components, which constitute a significant portion of the total electrolyser costs [1]. Atomic layer deposition (ALD) has emerged as a promising approach to overcome these challenges by offering unparalleled control over material deposition, allowing for the growth of ultra-thin films or nanoclusters with atomic precision. This technique not only maximizes material efficiency but also enhances device performance by minimizing waste.

ALD has demonstrated versatile applications in both catalyst coated membrane (CCM) and porous transport electrode (PTE) configurations. In CCM, platinum group catalysts can be efficiently coated on carbon powder using fluidized bed reactor ALD (FBR-ALD) and subsequently applied to membranes [2]. In a PTE, ultrahigh mass activities are achieved by atomically depositing Pt and Ir nanoclusters on titanium and graphite felts for anode and cathode sides, respectively [3]. Moreover, porous transport layers and bipolar plates, typically made from titanium and stainless steel, are coated with ultrafine Pt, Au, or nitride coatings to withstand high acidic and oxidation potentials [4]. Additionally, ALD is explored for fabricating support materials and providing porous and protective coatings in the form of oxides and metal organic frameworks (MOFs) [5,6]. These advancements highlight the potential of ALD in revolutionizing the efficiency, cost-effectiveness, and durability of PEM water electrolysers, thus paving the way for scalable and sustainable hydrogen production.

References

[1] Babic et al. (2017). Journal of the Electrochemical Society 164(4), F387 – F399.
[2] Lee et al. (2020). NPG Asia Materials. 12(40).
[3] Laube et al. (2021). International Journal of Hydrogen Energy 46(79), 38972 – 38982.
[4] Woo-Lee et al. (2020). Applied Surface Science 519, 146215.
[5] Li et al. (2024). Catalysis Science and Technology 14, 1328 – 1335.
[6] Xiao et al. (2024). ACS Applied Energy Materials 7(8), 3406 – 3413.

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Title: **[PP31]** Non-noble metal electrocatalysts for Hydrogen Evolution Reaction in PEM Water Electrolysis

Abstract: The Paris Climate Accords emphasize reducing greenhouse gas emissions, particularly carbon dioxide. Adopting hydrogen as an alternative fuel is promising, but developing its sustainable production with methods such as water electrolysis is needed to replace fossil fuel-dependent processes [1]. Proton-exchange membrane (PEM) water electrolysers offer an efficient solution for green hydrogen production but are hindered by their reliance on costly platinum group electrocatalysts.

This study explores the potential of replacing the state-of-the-art platinum electrocatalyst for the hydrogen evolution reaction (HER) with non-noble molybdenum phosphosulfides (MoP/S). Metal sulphides and phosphides, such as tungsten and molybdenum, offer cost-effective alternatives with unique mechanical, electronic, and chemical properties that are greatly beneficial for the HER [2]. While MoP/S typically shows lower catalytic activity than platinum, our research identifies four key strategies: (1) transforming the electrocatalyst into its metallic structural phase rather than stable semiconducting phase [3], (2) introducing sulphur vacancies to facilitate electron density transfer to the Mo atom [4], (3) maximizing edge sites to increase active sites [5], and (4) phosphorus doping to optimize proton adsorption [6], that can significantly enhance its performance. These strategies will first be tested in simple H-cell followed by an actual PEM cell, while comparing with the expensive platinum counterpart. Such advances could potentially position MoP/S as a promising, cost-effective alternative in electrocatalysis, paving the way for more sustainable hydrogen-production.

References

[1] Rogelj, Joeri et al. (2018). Intergovernmental Panel on Climate Change (IPCC).
[2] Nguyen, Tuan el al. (2023). Battery Energy, 2, 20220057.
[3] Voiry, Salehi et al. (2013). Nano Letters, 13(12), 6222–6227.
[4] Yin, Han et al. (2016). Journal of the American Chemical Society, 138(25), 7965–7972.
[5] Ho, Kim et al. (2021). ChemCatChem, 13(14), 3237–3246.
[6] Liu, Zhu et al. (2017). ACS Energy Letters, 2(4), 745–752.

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Title: **[PP32]** Gravity-Fed Laminar Electrolyser

Abstract: Alkaline water electrolysis is one of the most promising technologies for sustainable hydrogen production, but gas crossovers at low current densities limit its operating range, especially when paired with intermittent renewable energy sources. This study investigates the gravity-fed laminar electrolyser, designed to separate gas products and electrolyte flow at the production site and reduce gas crossovers to below the industrial safety limit of 2% at low current densities, addressing the limitations of traditional zero-gap electrolysers [1].

In-situ experiments were conducted using a custom-built prototype, focusing on performance and crossover concentration at low current densities. The study tested various electrode-membrane combinations (nickel meshes and felts paired with Zirfon 220 or Zirfon 500 membranes, and also in combination with ePTFE as the outermost layer), as well as three channel widths (1 mm, 0.7 mm, and 0.5 mm). The concentrations of hydrogen in oxygen (HTO) were measured using a gas chromatograph, while oxygen in hydrogen was determined with an oxygen sensor. The volumetric flow rate of the electrolyte (6M KOH) was measured using a flow meter. At the same time, the temperature was controlled through a heating plate and thermocouple, to ensure homogeneous temperature distribution along the bulk and the perimeter of the electrolyte reservoir a magnetic stirrer was used.

The experiments revealed that lower Reynolds numbers (closely interlinked with the electrolyte's viscosity, temperature and mass fraction [2]) due to the narrower channel widths, create a laminar flow regime that enhanced hydrogen convection, effectively minimizing crossover at low current densities. Furthermore, the thin channel also helped mitigate ohmic losses at higher polarisation levels. Among the tested electrode configurations, nickel mesh outperformed nickel felt due to its superior contact quality, open structure and ability to seep into the Zirfon membranes, which allowed hydrogen to escape more freely. Despite better performance, Zirfon 220 showed higher crossover concentrations, attributed to its higher porosity and diffusivity [3]. However, even thinner channels further curtailing electrolyte flow rates are expected to increase crossover due to the dominant role of diffusion in mass transfer at these rates. Moreover, temperature was found to be a key factor, as higher temperatures significantly reduced concentration overpotentials, enabling current density to start rising from a lower trigger voltage. Although this study validates the laminar electrolyser's potential in reducing gas crossovers at low current densities, the experiments were not conducted under industrial conditions and scale. Further tests are recommended.

References

[1] Trinke et al. - 2018 - Hydrogen Crossover in PEM and Alkaline Water Electrolysis
[2] Le Bideau et al. - 2019 - Review of Necessary Thermophysical Properties and their sensivities with temperature and electrolyte mass fractions for alkaline water electrolysis
[3] Schalenbach et al. - 2016 - Hydrogen Diffusivity and Electrolyte Permeability of the Zirfon PERL Separator for Alkaline Water Electrolysis

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Title: **[PP33]** Closed-Loop Recyclable Lignin-based Triboelectric Nanogenerators

Abstract: Triboelectric Nanogenerators (TENGs) are an emerging high-entropy mechanical energy harvesting device.[1] Compared with other nanogenerator devices, TENGs have higher energy conversion efficiency and output performance and can harvest random low-frequency micro energy from the environment. In addition, the materials that can be used to manufacture TENGs are widely selected, which has many advantages such as ease of manufacturing, diverse structures, low production cost, and environmental friendly.[2] TENGs excellent energy conversion efficiency can collect irregular and wasted energy signals in life, and convert various forms of mechanical energy into electrical energy and signals, such as human movement, wind, and blue energy. A multitude of different materials can be used for the synthesis of TENGs. such as PTFE, FEP, PDMS, and Kapton. However, under TENGs mode of operation as generators, TENGs are inevitably subjected to frequent external mechanical impact, resulting in structural defects in the material, affecting its output performance, and thus reducing the service life of TENGs. At the same time, current TENG materials rely on petrochemical products, and most of them are usually incinerated and landfilled after losing their use value, which also exacerbates the problems of resource shortage and environmental pollution. Lignin is considered one of the most abundant renewable sources of polyphenolic aromatic structural substances on Earth. Different types of lignin can be obtained by plant species and different lignin fractionation processes. Organosolv lignin (OSL) is an important candidate for the preparation of biomass chemicals and materials due to the lack of sulfur in its catalytic system, its high purity, and good solubility in organic solvents, make it suitable for synthetic reactions.[3] Covalent adaptable networks (CANs) are a type of polymer that represent a highly capable material, which dynamic covalent bonding in a cross-linked network enables to improve the material reprocessing in polymer applications.[4] Here, we explored the synthesis of vinylogous urethane cross-linked vitrimers from lignin, of which the properties can be tuned by adjusting the ratios of components to obtain a soft, elastic-flexible and brittle vitrimer films. Several to obtain a soft, elastic-flexible and brittle vitrimer films have triboelectric nanogenerator properties with the best performing material having an output voltage of 250 V under a load of 50 N, which creates the potential for simple and light mechanical power harvesters. The materials can be processed and recycled. The rate of decrosslinking can be controlled by temperature, acid content, cross-linking ratio and composition of the initial lignin and vinyl modifying material.

References

[1] T. Cheng, et al., Nature Reviews Methods Primers 2023, 3.
[2] S. Niu, Z. L. Wang, Nano Energy 2015, 14, 161-192.
[3] W. Schutyser, et al., Chemical Society Reviews 2018, 47, 852-908.
[4] M. A. Lucherelli, A. Duval, L. Avérous, Progress in Polymer Science 2022, 127.

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Title: [**PP34**] Unentangling PVC recycling: Challenges, Gaps, and Perspective

Abstract: In order to make better use of resources, recycling of plastics is not only desirable, but also required in the Netherlands starting from 2027 with new plastic products needing to contain 15 % recycled polymer [1]. Recycling of polyvinyl chloride (PVC) is a challenging affair and has not been solved, particularly with regard to mechanical recycling. Mechanical PVC recycling suffers from hydrochloric acid release, which occurs during (re-)heating. Another issue is the presence of legacy additives which have been banned by the European Commission's Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) legislation [2]. Legacy additives in PVC will continue to be a problem for PVC recycling for decades to come given that around half of produced PVC is applied in construction in products with multi-decade life-spans. In this work the challenges of mechanical PVC recycling are discussed alongside the general challenges of mechanical plastic recycling. Recent work from literature is shown and used to point out the gaps which need to be addressed in order for these methods to be suitable PVC recycling technologies. Lastly, a perspective is provided with a possible method to overcome the challenges of mechanical PVC recycling. It is argued that any PVC recycling method needs to be at least capable of removing the legacy additives, otherwise PVC recyclate is not allowed to be used in the EU. The technologies currently investigated in research are not capable of satisfying this demand, however the use of a processing agent which can both extract legacy additives and decrease processing temperature has the potential of alleviating these issues. As a result, mechanical recycling of PVC may become a possibility in the near future, which would allow PVC waste be handled in a much more circular fashion.

References

[1] R. Jager, J. Vlugter, and I. Gort, "Gevolgen Nationale Norm Circulaire Plastics," Sep. 2023. Accessed: May 31, 2024. [Online]. Available: https://www.rijksoverheid.nl/documenten/rapporten/2023/09/29/gevolgen-nationale- norm-circulaire-plastics

[2] "Commission Regulation (EU) 2023/923 of 3 May 2023 amending Annex XVII to Regulation (EC) No 1907/2006 of the European Parliament and of the Council as regards lead and its compounds in PVC," Official Journal of the European Union L 123, pp. 1–6, May 2023, Accessed: May 24, 2024. [Online]. Available: http://data.europa.eu/eli/reg/2023/923/oj

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Title: **[PP35]** Multifunctional Hydrogels for Underwater Motion Detection and Information Transmission

Abstract: Recent times have experienced a rapid expansion of flexible electronic devices, which are widely utilized in diverse applications including human motion detection, health monitoring, electronic skins, flexible sensors, and soft robotics. The considerable water content in hydrogels facilitates the transport of ions, while also providing properties similar to human tissues and other living organisms. These characteristics, make hydrogels a popular choice for wearable and flexible electronics.[1] However, due to the high hydrophilicity, hydrogels often experience unavoidable swelling in aqueous environments, leading to a significant decrease in mechanical strength, that is undesirable in numerous applications.[2] Furthermore, the swelling can diminish the conductivity of hydrogels, due to the dilution of the conductive network. To address such issues, considerable efforts have been dedicated to reducing swelling in hydrogels through the incorporation of hydrophobic segments,[3] increase of crosslinking density,[4] or simply using entirely hydrophobic environments. In this study, a physically cross-linked composite hydrogel is proposed, that is transparent, highly stretchable, anti- swelling, capable of autonomous self-healing, adhesive and anti-freezing. The hydrogel is synthesized through a simple one-step photopolymerization of acrylic acid (AA), [2-(methacryloyloxy) ethyl]dimethyl-(3-sulfopropyl) ammonium hydroxide (SBMA), and dodecyl acrylate (DA) in a novel deep eutectic solvent (DES)/H2O binary system. Dynamic physical interactions, including hydrophobic interaction, hydrogen bonding, and electrostatic interactions, confer remarkable transparency (92%), self-healing capability (up to 94%), self-adhesive to a wide array of substrates (91 to 199 kPa), high toughness (1.46 MJ m^{-3}), excellent elongation at break (up to 2064%), and resistance to swelling in water (equilibrium swelling ratio of 3% in water for 30 days) even in solutions at different pH (pH 1-11), and in other solvents. The incorporation of a DES contributes to exceptional anti-freezing performance, with a freezing point below -70 °C. Consequently, the transparent sensor achieves multifunctional sensing and human motion detection with high sensitivity and stability. Notably, the sensor demonstrates information transmission underwater through stretching and pressing, showcasing its immense potential in underwater flexible devices.

References

[1] Z. X. Wang, Z. J. Zhou, S. J. Wang, X. M. Yao, X. W. Han, W. T. Cao, J. W. Pu, Compos. Part B-Eng. 2022, 239, 109954
[2] X. Y. Dou, H. F. Wang, F. Yang, H. Shen, X. Wang, D. C. Wu, Adv. Sci. 2023, 10, 2206242.
[3] L. Han, M. H. Wang, L. O. Prieto-López, X. Deng, J. X. Cui, Adv. Funct. Mater. 2020, 30, 1907064. 4. S. Zhang, Y. L. Li, H. J. Zhang, G. J. Wang, H. Wei, X. Y. Zhang, N. Ma, Acs Mater. Lett. 2021, 3, 807.

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Title: **[PP36]** Design and development of bio-based amphiphilic polymers with antibacterial properties

Abstract: Antibiotic resistance has become an urgent issue in the global healthcare and agriculture fields. Meanwhile, the increasing emphasis on personal health and quality of life has led to a growing demand for novel and highly effective antibacterial materials in human society[1]. The amphiphilic antibacterial polymers synthesized by mimicking the function and molecular features of antibacterial peptides possess strongly active cationic and hydrophobic monomers[2]. Therefore, this project aims to synthesize novel polymeric agents with high antibacterial activity and low toxicity to host cells by utilizing bio-based chemicals (amino acids and tetrahydrogeraniol) as raw materials and to investigate the impact of different amino acid side chains (aliphatic/aromatic, positively charged) on the antibacterial activity of the synthesized amphiphilic antibacterial polymers. In this study, a library of amphiphilic copolymers was successfully synthesized using Reversible Addition Fragmentation chain Transfer polymerization (RAFT)[3].Specifically, all polymers were prepared with a target degree of polymerization (DPn) of 20 (with the Chain Transfer Agent (CTA) comprising 5% of the total molar amount of monomers), and included three components: 1) Cationic groups, represented by three amino acids with different side chains: alanine (with a methyl side chain), phenylalanine (with an aromatic phenyl ring), and lysine (with an amino positively charged side chain). 2) Hydrophobic monomer, derived from bio-based THG and modified with a double bond to form THGA. 3) End-groups, achieved by using different CTA: CDPA(with a long aliphatic chain). By adjusting the ratio of hydrophilic cationic monomers to hydrophobic monomers, a series of amphiphilic random copolymers with varying molar ratios between the two components were synthesized to study their structure-activity relationships. The antibacterial test results showed that for Gram-negative bacteria E.coli, higher hydrophilicity showed stronger antibacterial activity, and the sample with a Lys to THGA ratio of 9:1 had the strongest activity, with a MIC of 125 µg/ml. The results for other bacteria and cytotoxicity have not yet been completed.

References

[1] English, B. K.; Gaur, A. H. The use and abuse of antibiotics and the development of antibiotic resistance. Hot topics in infection and immunity in children VI 2010, 73-82.

[2] Takahashi, H.; Caputo, G. A.; Kuroda, K. Amphiphilic polymer therapeutics: an alternative platform in the fight against antibiotic resistant bacteria. Biomaterials Science 2021, 9 (8), 2758-2767.

[3] Palermo, E. F.; Vemparala, S.; Kuroda, K. Cationic spacer arm design strategy for control of antimicrobial activity and conformation of amphiphilic methacrylate random copolymers. Biomacromolecules 2012, 13 (5), 1632-1641.

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Title: **[PP37]** Inverse gas chromatography, a new technique to investigate surfaces for porous media applications

Abstract: Porous materials are utilized in process engineering in a wide range of applications, e.g. catalysis support, filtration or electrodes. One of the advantages porous media offer is their high specific surface area allowing for intensified fluid-fluid and fluid-solid contact. Often, it is this property, which makes the process performance economic.

However, challenges remain in the design and manufacturing of the porous structure. Their development requires substantial trial and error before a satisfying solution is found. One challenge hereby is the scale-dependent structural and chemical heterogeneity of the internal surface of the porous substrate.

Inverse gas chromatography (iGC) is a powerful, sensitive, and relatively fast technique for characterizing the physicochemical properties of porous media such as BET surface area and surface energy distribution [1]. In this technique, probe molecules in the form of gas, are injected into a column packed with the porous sample under investigation. The probe molecules pass through the column and interact with the porous material before their retention is recorded by an flame ionization detector. By combining information on the retention times for different probing molecules we can infer the properties of the internal surface in a porous substrate, e.g. polar and non-polar surface energies. Measurements at elevated temperatures and humid conditions allow the investigation of materials at operational conditions and further provide the potential to map surface energies in relation to pore sizes [2,3,4].

In this study, we present how the molecular properties determined with iGC are linked to macroscopic responses for model glass bead-pack and PTFE systems with different modifications. The data provides a first proof of concept motivating to further explore the possibility of iGC to study surface characteristics of porous substrates during manufacturing and operation aiding future design decisions.

References

[1] Thielmann F., Journal of Chromatography A, 2004, 1037, 115-123.

[2] Strzemiecka B., Kołodziejek J., Kasperkowiak M., Voelkel A., Journal of Chromatography A, 2013, 1071, 201-206.

[3] Sheng, Q., et al, Science Report, 2016, 6, 30764.

[4] Rücker, M. et al, 'Relationship between wetting and capillary pressure in a crude oil/brine/rock system: From nano-scale

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Title: **[PP38]** Experimental characterization of co-adsorption kinetics and thermodynamics in solid sorbents for DAC

Abstract: Direct Air Capture (DAC) is a promising method of mitigating CO_2 emissions so that climate goals such as the Paris Agreement can be achieved. While large point-sources such as cement factories have high CO_2 concentrations in their flue gases and are therefore easier to handle, this does not mitigate the CO_2 emissions of smaller, distributed sources such as in the transportation sector. For this reason, DAC is considered to be promising, as it collects CO_2 from ambient air and is thus not geographically restricted, which contributes to the economic viability of its implementation. Furthermore, while the presence of water in the form of moisture results in lower CO_2 adsorption capacities in many other sorbent types such as zeolites, amine-functionalized solid sorbents display increased adsorption in humid conditions due to co-adsorption. This would be beneficial in real-life applications, as ambient air generally contains moisture at higher concentration than CO_2. However, additional data regarding the kinetics and thermodynamics of this co-adsorption phenomenon is required to provide a clear indication of the viability of large-scale implementation of this method for decarbonization.

In this study, we present our experimental findings of TGA and breakthrough measurements pertaining to the co-adsorption phenomenon. The combination of these two measurement techniques allows for an in-depth analysis, where the effect of temperature, CO_2 partial pressure, and relative humidity on the kinetics and thermodynamics of co-adsorption will be investigated. Furthermore, general characterization of the solid sorbent such as particle size distribution, BET surface area, and density is performed in order to model the reactor and allow for future economic analysis.

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Title: **[PP39]** Hydrogenation of bio-derived aldehydes over N-doped C-supported cobalt catalysts

Abstract: Selective hydrogenation is a crucial process in the synthesis of chemical intermediates.[1, 2] Here, we report the efficient hydrogenation of 5-hydroxymethylfurfural (HMF) to 2,5-bishydroxymethylfuran (BHMF) over N-doped C-supported cobalt catalysts with the core-shell structure (CoOx@Co-NC) derived from ZIF-67. Pre-treatment of the catalyst through oxidative treatment at different temperatures greatly affected the catalytic activity. The catalyst that was activated by oxidative pretreatment at 200 °C exhibited the best catalytic performance in HMF hydrogenation to BHMF, affording 93.2% HMF conversion and 99% BHMF selectivity, approximately 30% higher than the non- oxidized catalyst (reaction conditions: 100 °C, 20 min). Complete HMF conversion and high BHMF selectivity were obtained at reaction temperatures up to 120°C, either at room temperature within 8 hours or at 120 °C within 30 minutes. The enhanced activity at low temperatures was attributed to the interaction between CoOOH and Co_3O_4 with high-valence cobalt on the N-doped carbon support, as evidenced by various characterization techniques. Overall, this study established the correlation between surface oxidation and catalytic performance in hydrogenation reactions, providing valuable insight in enhancing the performance of catalysts.

[1] T. Wang, W. Xie, Y. Pang, W. Qiu, Y. Feng, X. Li, J. Wei, X. Tang and L. Lin, ChemSusChem, 2022, 15, e202200186.
[2] Y. Feng, S. Long, X. Tang, Y. Sun, R. Luque, X. Zeng and L. Lin, Chem Soc Rev, 2021, 50, 6042-6093

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Title: **[PP40]** Effect of molecular weight on transport limitation in Plastic Hydrogenolysis

Abstract: As of 2024, global plastic production has surpassed 400 million tons, yet only 9% of plastic waste undergoes recycling [1]. Conventional disposal methods, such as landfilling and incineration, are increasingly criticized for their environmental impact, including significant global warming potential and the contamination of soil and groundwater [2]. Mechanical recycling, a widely practiced downcycling approach, results in the degradation of material properties, limiting its effectiveness and sustainability [3]. In contrast, chemical upcycling has gained attention as a promising strategy to convert plastic waste into value-added chemicals, thereby offering a more sustainable solution [3].

Among the chemical upcycling techniques, pyrolysis, hydrocracking, and hydrogenolysis are commonly explored. However, both pyrolysis and hydrocracking produce a broad spectrum of products with poor selectivity, leading to high separation costs thus reducing their scalability potential [4]. Hydrogenolysis, on the other hand, demonstrates higher selectivity towards liquid hydrocarbons in the C5-C35 range, which are suitable as alternative fuels [5]. Despite its advantages, hydrogenolysis is hindered by the longer reaction times required for complete conversion, often extending up to 96 hours. This prolonged reaction time is primarily attributed to mass transfer limitations, driven by the high viscosity of molten plastics and the significantly lower solubility of hydrogen—approximately 10^6 times lower than in other liquid hydrocarbons. The viscosity and hydrogen solubility of polymers are closely related to their molecular weight, suggesting a strong correlation between molecular weight and mass transfer limitations in hydrogenolysis. This research focuses on investigating the effect of molecular weight on the hydrogenolysis of plastics by utilizing three reactants with varying molecular weights: n-hexadecane, paraffin wax, and low-density polyethylene (LDPE). A Ru/SiO_2 catalyst with ruthenium particle sizes of approximately 15 nm is employed to conduct the reactions in a batch reactor.

This study aims to elucidate the relationship between polymer molecular weight and the associated transport limitations during hydrogenolysis, providing insights that could enhance the scalability and efficiency of chemical upcycling processes. Understanding these dynamics is crucial for optimizing reaction conditions and developing more effective strategies for the large-scale conversion of plastic waste into valuable chemical products.

References

[1] C. Wang et al., “Polyethylene Hydrogenolysis at Mild Conditions over Ruthenium on Tungstated Zirconia,” JACS Au, vol. 1, no. 9, pp. 1422–1434, Sep. 2021, doi: 10.1021/JACSAU.1C00200/SUPPL_FILE/AU1C00200_SI_002.ZIP.

[2] J. P. Lange, S. R. A. Kersten, S. De Meester, M. C. P. van Eijk, and K. Ragaert, “Plastic recycling stripped naked – from circular product to circular industry with recycling cascade,” ChemSusChem, p. e202301320, 2024, doi: 10.1002/CSSC.202301320.

[3] R. Balu, N. K. Dutta, and N. Roy Choudhury, “Plastic Waste Upcycling: A Sustainable Solution for Waste Management, Product Development, and Circular Economy,” Polymers (Basel), vol. 14, no. 22, Nov. 2022, doi: 10.3390/POLYM14224788.

[4] Q. Qian and J. Ren, “From plastic waste to potential wealth: Upcycling technologies, process synthesis, assessment and optimization,” Science of The Total Environment, vol. 907, p. 167897, Jan. 2024, doi: 10.1016/J.SCITOTENV.2023.167897.

[5] U. R. Gracida-Alvarez, O. Winjobi, J. C. Sacramento-Rivero, and D. R. Shonnard, “System Analyses of High-Value Chemicals and Fuels from a Waste High-Density Polyethylene Refinery. Part 2: Carbon Footprint Analysis and Regional Electricity Effects,” ACS Sustain Chem Eng, vol. 7, no. 22, pp. 18267–18278, Nov. 2019, doi: 10.1021/ACSSUSCHEMENG.9B04764/ASSET/IMAGES/LARGE/SC9B04764_0009.JPEG

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Title: **[PP41]** Cs-enhanced Ru-based catalysts for low-temperature ammonia decomposition

Abstract: Hydrogen can be seen as a promising energy vector in the framework of energy transition as, on one side, it can be produced through water electrolysis employing renewable energy sources and, on the other side, the only product emitted from its combustion is water. Moreover, ammonia can be considered a suitable hydrogen carrier as it has a high hydrogen content, it contains no carbon and it is characterized by an easier storage and transportation than for pure hydrogen [1]. The efficient utilization of ammonia as a hydrogen storage medium must address efficiently the step of ammonia decomposition, an endothermic equilibrium reaction typically conducted in a temperature range of 450 – 550°C and a pressure range of 1 – 3 bar [2], and the separation and purification of the resulting mixture. This study investigates the impact of ruthenium loading and the effect of cesium promotion on the catalytic performance of the synthesized catalysts for ammonia decomposition. Ru/CeO_2 (Ru 3 – 7 wt%) and Cs-Ru/CeO_2 (Ru 5 wt% ,Cs/Ru = 0 – 2 w/w) catalysts were prepared. For each catalyst, a solution composed by all the metal precursor salts was prepared using ethylene glycol as solvent. The solution was placed in a three-neck round bottom flask connected to a condenser, employed to cool down and condense the vapors and recycle them as liquids back into the synthesis vessel. The system was heated up to 110°C, then kept at this temperature for 2 hours to obtain a homogeneous dark colloidal solution, after which the mixture was cooled down naturally. Then, a KOH solution was slowly added to the mixture and the resulting gel was aged and washed with ultrapure water. Finally, the catalyst was dried and then calcined at 550°C for 4 hours. Several characterization techniques were utilized to comprehensively analyze the structural and surface properties of the catalysts. The results show that the best performance can be achieved employing 5% ruthenium loading, reaching equilibrium ammonia conversion already between 375 and 400°C at ambient pressure. The addition of cesium to the catalytic formulation resulted in a significant improvement. More specifically, at 350°C the conversion increased approximately 33% and the equilibrium curve was already approached at 375°C. These findings offer valuable insights into the mechanistic aspects of Cs-enhanced Ru-based catalysts and their potential applications in sustainable hydrogen production. Similar results in literature can be found only for reaction systems employing very diluted feeding streams [3].

References

[1] Lucentini, I; et al. Catalytic ammonia decomposition for hydrogen production on Ni, Ru and Ni single bond Ru supported on CeO2. Int. J. Hydrogen Energy 2019, 44 , 12693 – 12707.
[2] Cechetto, V; et al. Gallucci, F. Ultra-pure hydrogen production via ammonia decomposition in a catalytic membrane reactor. Int. J. Hydrogen Energy 2022, 44, 21220 – 21230.
[3] Chen, C.; et al. Ru-Based Catalysts for Ammonia Decomposition: A Mini-Review. Energy Fuels 2021, 35, 11693 – 11706.

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Title: **[PP42]** Catalytic conversion of lower olefins to BTX range of aromatics using zeolite-based catalysts

Abstract: Aromatics, especially benzene, toluene, and xylenes (BTX), are an important class of platform chemicals that are used extensively for the production of specialty chemicals, paints, polymers etc. Considering the need to transit towards more circular alternative carbon feedstocks, production of BTX from lower olefins offers a viable solution as these olefins can be derived easily from biomass and waste plastics.[1, 2] Aromatization of olefins is typically carried out at ambient pressure and temperatures between 673 and 773 K using a zeolite- based catalyst. The selectivity towards BTX aromatics can be improved by incorporating promoters such as Ga, Zn, Ag etc. into the zeolite.[3, 4] In this work, we first identified the preferred olefin feed, ethene or propene, for BTX production in a fixed-bed reactor using commercial H-ZSM-5 (Si/Al = 23) and Ga-modified ZSM-5 catalysts. At 773 K, 1 bar, 45 %v. olefin, 6.75 h^{-1}, aromatization of propene over Ga- ZSM-5 catalyst exhibited higher BTX selectivity of 55% and resulted in slower catalyst deactivation compared to ethene aromatization. These results suggest that the overall BTX yields can be improved if propene can be selectively produced during pyrolysis and additionally be converted in the recycle gas stream of biomass/ plastics pyrolysis. Considering the commercial importance of p-xylene, we aimed at improving its selectivity using propene as feed by further modifying the Ga-ZSM-5 catalyst. Two different surface-modification techniques were employed on the catalyst and upon modification, p-xylene selectivity was improved. Further structure-performance relations of the aromatization of propylene towards p-xylene will be discussed in this contribution.

References:

[1] Netsch, N.; Vogt, J.; Richter, F.; Straczewski, G.; Mannebach, G.; Fraaije, V.; Tavakkol, S.; Mihan, S.; Stapf, D., Chemical Recycling of Polyolefinic Waste to Light Olefins by Catalytic Pyrolysis. Chemie Ingenieur Technik 2023, 95 (8), 1305-1313.

[2] Zacharopoulou, V.; Lemonidou, A., Olefins from Biomass Intermediates: A Review. Catalysts 2017, 8 (1).

[3] Uslamin, E. A.; Saito, H.; Kosinov, N.; Pidko, E.; Sekine, Y.; Hensen, E. J. M., Aromatization of ethylene over zeolite-based catalysts. Catalysis Science & Technology 2020, 10 (9), 2774-2785.

[4] Butolia, P. S.; Xi, X.; Winkelman, J. G. M.; Stuart, M. C. A.; van Akker, M.; Heeres, A.; Heeres, H. J.; Xie, J., Advantages of Producing Aromatics from Propene over Ethene Using Zeolite-Based Catalysts. Chemie Ingenieur Technik 2022, 94 (11), 1845-1852.

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Title: **[PP43]** Methodology for Bubble Formation and Characterization in Viscous Media for Chemical Reactions

Abstract: Formation of micro-sized bubbles in highly viscous liquids is challenging due to the high share rates required to form the bubbles. This is particularly critical when conducting catalytic conversion of plastic waste in the molten phase in which it is essential to ensure proper mass transport of gaseous reactants with the liquid plastics consequently improving the reaction time and conversion[1,2]. Here, it is germane to understand the interplay between mass transfer and fluid dynamics with chemical reactions for plastic upcycling.

To address this issue, the present study presents a methodology for investigating bubble formation in viscous media. Computational Fluid Dynamics (CFD) simulations are conducted within COMSOL to establish fundamental relationships between the fluid mechanics involved in bubble formation. The complex interactions at the interface and chemical reactions are often neglected [3,4]. For this reason, in this study, we will establish the basis for the introduction of chemical reactions of plastic waste chemical conversion at the gas-liquid interface of micro-bubbles.

Two distinct flow geometries of microfluidic devices are studied namely the co-flow and the focus flow. The geometries are relevant in controlling bubble formation at the microscale. Precise control of flow conditions is important for understanding bubble generation. By systematically varying the flow rate, viscosity, and temperature, specific conditions of bubble formation are identified. Using these conditions, phase diagrams are reconstructed where the regimes of bubble formation are indicated.

The results imply that the formation of bubbles is mainly controlled by the flow conditions of the gas and liquid phase and the properties of the media, such as viscosity, density and surface tension. The results have significant implications for industrial-scale applications, that are mass transport limited due to the high viscosity of the chemical species. Bubble formation in viscous media can be applied to improve the interfacial contact between the liquid and gas phases.

References

[1] Mehdi, S., Billet, A. M., Chughtai, I. R. & Inayat, M. H. Asia-Pacific Journal of Chemical Engineering 8, 931–939 (2013).

[2] Aoki, J., Hayashi, K., Hosokawa, S. & Tomiyama, Chem Eng Technol 38, 1955–1964 (2015).

[3] Gerlach, D., Alleborn, N., Buwa, V. & Durst, Chem Eng Sci 62, 2109– 2125 (2007).

[4] Chakraborty, I., Biswas, G. & Ghoshdastidar, P. S. Int J Heat Mass Transf 54, 4673–4688 (2011).

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Title: **[PP44]** Electrodialysis Based Membrane Assisted Electro-Osmotic Dewatering of Biomass

Abstract: In the quest for new sustainable processes to facilitate the electrification of industrial operations, such as biomass drying, electrochemical-based technologies play a crucial role. Numerous efforts have been made to develop energy storage and conversion technologies to reduce dependence on fossil fuels, alongside the adoption of renewable energies. Despite these efforts, energy-intensive thermal drying processes require attention to identify an alternative electrified solution that can shrink the global carbon footprint. In this context, we will discuss our recent efforts in utilizing an electrodialysis-based, ion exchange membrane assisted, non

thermal electro-dewatering process as an alternative solution to thermal drying processes. Typically, electroosmotic water transport in electrodialysis systems is considered detrimental to the desalination processes [1,2]. However, we can leverage this undesirable process to remove excess water present in the biomass samples. We will explore the possibilities and explain the role of the electrodes, membranes, and ions present in the feed, as well as their influence on the biomass dewatering process.

References
[1] H. Strathmann, Electrodialysis, a mature technology with a multitude of new applications. Desalination 264 (2010) 268-288.
[2] M. Tedesco, H. V. M. Hamelers, P. M. Biesheuvel, Nernst-Plank transport theory for (reverse) electrodialysis: II. Effect of water transport through ion-exchange membranes, Journal of Membrane Science 531 (2017) 172-182.

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Title: **[PP45]** Isolation of anacardic acid from natural cashew nutshell liquid using ion exchange resins

Abstract: The cashew (Anacardium occidentale) holds a significant position in global agriculture and trade, with approximately 5.7 million hectares worldwide dedicated to cashew plantations [1]. In 2022, Europe emerged as the largest importer of cashew nut kernels, reflecting a trade value of approximately 1.5 billion euros with an estimated annual growth rate of 3-5% [2].

Cashew Nut Shell (CNS) is a waste generated in the production of edible cashew nut. CNS contains circa 30-35% brown viscous liquid, called Cashew Nut Shell Liquid (CNSL), which is a natural resin containing valuable components, for example, cardanol, cardol and anacardic acid. Particularly anacardic acid (AA), a phenolic compound, is valued for its anti-bacterial, anti-fungal, anti-tumor, anti-inflammatory, insecticidal, and fungicidal properties.

However, industrial separation processes for high-purity anacardic acids are challenging due to the presence of phenolic components (cardols and cardanols) with similar chemical properties. In this work, the feasibility to separate and purify anacardic acid by resin adsorption has been investigated.

The experimental results showed that a maximum anacardic acid adsorption capacity of 581.8 mg/g resin can be obtained using Mitsubishi Dianion WA30 resin. The obtained equilibrium information was used as input in a dynamic column model and the modelling results were compared with experimental results, showing good agreement. The model will be further applied for a large-scale adsorption process design to recover anarcardic acid from CNSL.

References

[1] Adekanbi, M. L., & Olugasa, T. T. (2022). Utilizing cashew nut shell liquid for the sustainable production of biodiesel: A comprehensive review. Cleaner Chemical Engineering, 4, 100085.

[2] A. Global, "The European market potential for cashew nuts," 25 January 2024. [Online]. Available: https://www.cbi.eu/market-information/processed-fruit-vegetables-edible-nuts/cashew-nuts/market-potential.

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Title: **[PP46]** Modelling CO_2 adsorption for Direct Air Capture using Multiphysics CFD

Abstract: Direct air capture (DAC) is an emerging technology to remove CO_2 from the atmosphere, helping to quicker reach net zero emissions and limit global warming. In this work, we focus on solid-sorbent DAC, where air is flown through a sorbent structure, which is subsequentially regenerated at elevated temperature and/or reduced pressure. One of the major challenges associated this technology are the energy losses associated with flow, heat and mass transfer. Simplified 1D linear driving force models fail to properly predict these phenomena in complex sorbent/contactor geometries as well as the local and temporal effects and variance of heat and mass transfer. The poster will show our progress in modelling the heat and mass transport during the adsorption stage of the process.

We assess the heat and mass transfer phenomena by making use of multiphysics and multiphase direct numerical simulation at sorbent scale, using a versatile Open FOAM solver. We consider a porous amine functionalized materials, as they have been widely tested in various experiments [1]. The gas phase is modelled through a compressible flow solver, while the sorbent is modelled as a homogenous solid, where pore diffusion and reaction models account for adsorption in the pores. Modelling the thermodynamic and chemical equilibria and reaction kinetics allows for accurate quantitative prediction of concentration and temperature profiles in complex sorbent structures. Accurate tracking of concentrations of absorbed CO_2 and H_2O allows us to assess sorbent performance under various humidity levels and temperatures, accounting for seasonal variations. This methodology is key for to the design of more sophisticated DAC contactors and processes.

The presented simulations cases represent porous silica monoliths with varying amine loadings and geometries. Our approach allows us to examine the effect of these parameters on capacity and adsorption rate. These results are used for assessing the performance of sorbent materials under various operational conditions. This poster will shed light on how monolith structures, amine loadings determine the suitability of a given configuration for a given environment.

References

[1] Y. Miao, Z. He, X. Zhu, D. Izikowitz, and J. Li, “Operating temperatures affect direct air capture of CO_2 in polyamine-loaded mesoporous silica,” issn:13858947. doi: 10.1016/j.cej.2021.131875.

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Title: **[PP47]** Electrical drying of biomass by electro-osmosis and electrohydrodynamic drying: effect of internal transport phenomena

Abstract: The world is transitioning towards renewable and biobased materials. These streams contain large amounts of water reaching 95 % and require dewatering. Current drying technologies account for 15-25 % of all energy consumed in industry and most of this consumption is for drying of biomass in the conversion process into food or bio-based products. The development of non-thermal processes employing other driving forces, such as electric fields, would make it possible to strongly reduce the energy consumption of dewatering and concentration. At the same time, operation at low temperatures also means better quality of the dried materials and that more sensitive materials can be treated.

The de-watering technologies of electro-osmosis (EO) and electrohydrodynamic (EHD) drying both feature an applied electric field across a biomass sample, and presence of charged species inside the biomass matrix, which induce the movement of liquid inside the pores of biomass. Previous research has proven the feasibility and advantages of these technologies in terms of product quality and energy consumption. However, a better fundamental understanding of the transport mechanisms inside the biomass is required to enable the industrial application of these methods. To bridge this gap, we elucidate electrically induced water transport mechanisms in biomass as a function of its microstructure and properties, by combining micro-scale experiments and multi-physics modelling.

We use micromodels to visualize the transport of water induced by the applied electric field and study the effect of the medium geometry and properties. Multi-physics modelling enables us to evaluate the effect of matrix properties on the internal electric field for different microstructures. This combined approach can help evaluate which matrices dry more effectively for the sample applied voltage. The multi-physics model validated against experiments in micromodels can ultimately be applied to predict the electrically induced water removal performance in more realistic biomass models.

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Title: **[PP48]** Development of porous carbon materials for methane capture from diluted streams

Abstract: Methane (CH4) is the second largest contributor to global warming after carbon monoxide (CO_2) and, on a 100 year timescale, has an 84 times greater global warming potential than CO_2. More specifically, the emissions of CH_4 from the livestock sector have a huge environmental impact that may also affect the health of farm workers, animals, and the neighboring communities [1]. A possible solution to reduce CH_4 emissions in the atmosphere from the livestock sector and, therefore, reduce global warming and its dramatic consequences, is to directly remove CH_4 through tailored sorbents. In this overview, porous carbon materials might be an interesting option due to the low price, excellent chemical stability, low cost, and ease of production.

In a four neck round bottom flask, the starting amines (aniline, cyclohexylamine, benzylamine, propylamine) were added to melted phenol and the mixture was stirred. Then, formaldehyde was added dropwise while continuously stirring. The obtained mixture was kept under mixing for the fixed period defined for polymerization. The as-synthesized product was purified and dried under vacuum at 40 °C. The synthesized polybenzoxazines have been characterized through TGA-MS under nitrogen flow with a heating ramp of 20°C min-1 to investigate the most suitable carbonization temperature and qualify the evolved gas products. The relative intensity as a function of temperature, for several mass-to-charge ratios (m/z) has been studied for the polymer obtained with the addition of cyclohexylamine and reported in Figure 1.

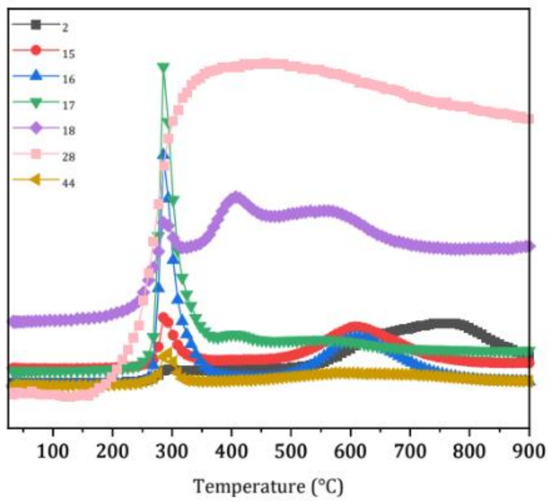

Figure 1. Relative intensity as a function of temperature.

Finally, the lab-scale fixed-bed adsorption experiments were performed in the Autochem II column (Micrometrics ®), whose diameter is more than at least seven times the adsorbent particle diameter, thus, it has no significant adverse effect on the breakthrough curves. Before the tests, the samples were degassed in-situ at 400°C to remove undesirable compounds possibly present on the surface of the material. After degassing, the adsorption was performed under nitrogen flow reaching the set temperature, waiting for the stabilization of the signal, and switching to the mixture containing 1% methane in nitrogen. The TCD signal was recorded over time, and it provides information on the methane concentration at the outlet of the packed bed of sorbent, thus from the TCD signal recorded during adsorption a breakthrough curve was obtained. From the breakthrough curve, for each sample, the adsorption capacity was calculated. The best results were achieved with benzylamine based polymer (adsorption capacity = 2.68 mmol g^{-1}).

Acknowledgements

The work is part of the project “Removing non-CO_2 greenhouse gas emissions to support ambitious climate transitions (REPAIR)” (Project number: 101069905) funded by the European Commission via the European Climate, Infrastructure and Environment Executive Agency (CINEA) within the Horizon Europe framework.

References

[1] N. M. Ngwabie, K. H. Jeppsson, S. Nimmermark, C. Swensson, and G. Gustafsson, “Multi-location measurements of greenhouse gases and emission rates of methane and ammonia from a naturally-ventilated barn for dairy cows,” Biosyst. Eng., vol.103, no.1, pp.68–77, 2009, doi: 10.1016/j.biosystemseng.2009.02.004.

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Title: **[PP49]** Thin-film-composite anion exchange membranes for increased OH- selectivity in CO_2 -electrolysis

Abstract: Ion exchange membranes (IEMs) play a pivotal role in the energy transition, to recover valuable products and to separate reactions for synthesis of sustainable fuels and chemicals. This includes technologies such as electrodialysis and electrolysis. Intensive research on materials for IEMs identified a trade-off between selectivity and permeance by charge density tuning, thereby intrinsically challenging to improve both properties.

Thin-film-composite (TFC) IEMs recently have been successfully applied for specialty separations. For example, membranes are coated with polymers containing opposite charge as the bulk layer, to achieve monovalent selectivity. Besides monovalent selectivity, cation-exchange-membranes (CEM) implementing this concept also demonstrate higher co-/counter-ion selectivity.1,2 However, none of these works targets OH- selectivity, anion/cation selectivity, water management or catalyst interaction. Research in our lab revealed that coating the supporting layer of a standard reverse osmosis (RO) membrane with a ionomer solution yields a highly selective TFC anion exchange membrane (AEM) which blocks all larger counter ions except for the smallest one: OH-

TFC membranes have been fabricated by applying liquid Sustainion® ionomer on the supporting back layer of a commercially available reverse osmosis (RO) membrane (BW30, FilmTec TM) by a very simple drop-casting method. The ionomer solution is applied and held in place by a plastic frame until the solvent evaporates. Afterwards, the membrane is dried at 40 °C in an oven. The conductive ionomer back layer provides conductivity while the polyamide layer provides size selectivity for larger anions such as (bi)carbonates while the smallest ions (namely OHand H+) can still pass. We choose this approach because previous attempts to coat a commercially available AEM with a size selective polyamide layer by using interfacial polymerization proved to be challenging.

Our proof-of-concept demonstrates a successful thin-film composite membrane made from a commercially available RO membrane. We observed a significant higher permeance of OHthan of bicarbonate. The results of these experiments and the implications of the results will be presented in form of a poster.

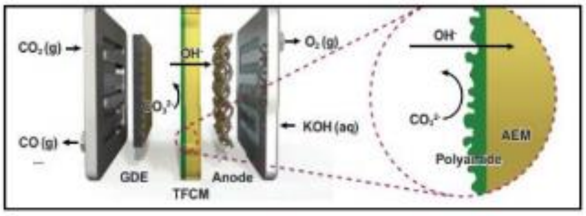

Figure 1: Concept of a size selective TFC anion exchange membrane in CO_2-electrolysis

References
[1] Wang, W. et al, Journal of Membrane Science, 2019. 58
[2] 2: p. 236-245 2. Hou, L. et al, Journal of Membrane Science, 2018. 557: p. 49-57.

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Title: **[PP50]** Bio-based Solvents for Circular Poly Vinyl Chloride Processing

Abstract: Plastic recycling has captured significant attention, instead of incinerating them at the end of their use phase, polymers can be a valuable resource for new products. Poly vinyl chloride (PVC) is a thermoplastic for wide applications. Additives such as thermal stabilizers and plasticizers are added to tune PVC properties to meet the requirements for their application. Dissolution recycling is a promising recycling technology that aims at maintaining the PVC molecules in their polymeric state. A suitable solvent dissolves PVC and some additives, while other additives do not dissolve. After filtering off the insoluble, the polymer should be fractionated from the solvent and other dissolved species. This fractionation is very important due to stricter limits on certain additives in plastic products [1]. Upon recycling, removal of such banned species to below the legal limits must thus be realized.

For dissolution-based recycling, the solvent is important and determines the fractionation strategies window. Because of the potential environmental impact of traditional solvents for a wide range of applications, more environmentally friendly solvents have been investigated [2]. Cyrene is a polar aprotic biobased solvent reported for several applications as environmentally friendly alternative to N-methyl-2-pyrrolidone, a commonly used solvent [3]. Similar to Cyrene, -valerolactone (GLV) is a biobased solvent and in this work, Cyrene and GVL have been studied for dissolving pure PVC, and PVC pipe materials and downstream fractionation of the PVC and other ingredients of the pipes. Mixtures of Cyrene or GVL with (2-methylhydrofuran) 2-MTHF, a bio-based solvent, and MEK, which is used in Vinyloop process, were studied alongside pure solvents. Various temperatures and concentrations of PVC (PVC pipe and Pure PVC) were studied and solubility and viscosity depended heavily on these parameters. The results indicated that the mixtures containing MEK or 2-MTHF demonstrate higher solubility compared to pure solvents at lower temperatures. Both GVL/2-MTHF and Cyrene/2-MTHF mixtures show promise as solvents for PVC dissolution.

References

[1] K. Lewandowski and K. Skórczewska, “A Brief Review of Poly(Vinyl Chloride) (PVC) Recycling,” Polymers, vol. 14, no. 15. MDPI, Aug. 01, 2022. doi: 10.3390/polym14153035.
[2] Z. Ait-Touchente, M. Khellaf, G. Raffin, N. Lebaz, and A. Elaissari, “Recent advances in polyvinyl chloride (PVC) recycling,” Polymers for Advanced Technologies, vol. 35, no. 1. John Wiley and Sons Ltd, Jan. 01, 2024. doi: 10.1002/pat.6228.
[3] R. A. Milescu et al., “Polymer Chemistry Applications of Cyrene and its Derivative Cygnet 0.0 as Safer Replacements for Polar Aprotic Solvents,” ChemSusChem, vol. 14, no. 16, pp. 3367–3381, Aug. 2021, doi: 10.1002/cssc.202101125.

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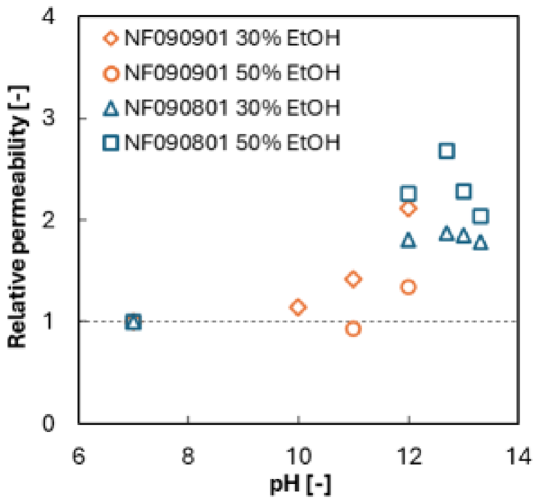
Title: **[PP51]** Investigating the performance of commercially available nanofiltration membranes in alcohol-water mixtures at high pH

Abstract: The development of nanofiltration (NF) membranes for alcohol-water media has led to multiple applications in the food, pharmaceutical and chemical industries. Alkaline-resistant NF membranes are used in these industries as well [1,2]. However, the application of NF membranes for the purification of alcohol-water media at alkaline conditions is still a challenge. Traditional polyamide thin-film composite membranes, commonly used for applications involving alcohol-water mixtures [3], are not stable at high pH [4,5], while the performance of alkaline-resistant NF membranes for alcohol-containing alkaline solutions is yet unknown [3]. In the Recircanol project, the influence of alcohol-alkaline mixtures on the properties, performance and stability of commercial NF membranes is being investigated.

First results indicate that for SolSep membranes NF090101 and NF090801 the permeability for ethanol-water mixtures containing either 30 wt% or 50 wt% ethanol (EtOH) and having a pH ≥ 11 is higher than that for similar mixtures at a pH = 7. Whether this increase in permeability is caused by membrane stability or by changing membrane properties at high pH conditions has not yet been established. More experiments will be performed to determine the effect of pH on membrane permeability and solutes retention, and to unravel the underlying mechanisms.

The final results of this project are expected to lead to a better understanding of how the morphology and performance of NF membranes will change when working with alcohol- water mixtures at high pH. This improved understanding is expected to support membrane manufacturers in improving their products and expanding their application portfolio.



References

[1] M.P. Belleville et al. (2021). Nanofiltration in the food industry. Nanofiltration: Principles, Applications, and New Materials, 2, 499-542.

[2] M. Kyburz et al. (2021). Nanofiltration in the chemical processing industry. Nanofiltration: Principles, Applications, and New Materials, 2, 543-597.

[3] A. El Fadil et al. (2024). Strong Impact of Exposure to Water/Solvent Mixtures on Permeance of Nanofiltration Membranes. J. Membr. Sci., 699, 122651

[4] W. Cheng et al. (2023). Oxidation Resistances of Polyamide Nanofiltration Membranes to Hydroxyl and Sulfate Radicals. J. Membr. Sci., 666, 121156.

[5] G. Bargeman (2021). Recent developments in the preparation of improved nanofiltration membranes for extreme pH conditions. Sep. Purif. Technol., 279, 119725.

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Title: **[PP52]** Design and scale-up of membrane reactor for ammonia synthesis

Abstract: The outstanding properties and features of hydrogen (H_2) make it a very promising energy carrier and fuel, although it is not naturally available in a ready-to-use form. [1] However, H_2 suffers a disadvantage due to its low volumetric energy density, which poses storage challenges. Ammonia (NH_3) is highly valued as a potential H_2 storage solution. It has in fact high H_2 density (17.8 wt%), and offers high flexibility in its utilization, including mobile and stationary applications. Moreover, its stability for long-term storage and transportation, enables NH3 to meet the demand of energy storage over time (stationary energy storage) and in space (energy export and import). [2] The system design of the NH_3 synthesis reactor poses a challenge due to the harsh reactor requirements, namely, a high inlet temperature to achieve high reaction rate and high pressure to achieve a high equilibrium conversion. Membrane operations offer intrinsic advantages, including efficiency, high selectivity and permeability for the transport of specific components, easy control and scale-up. [3] These characteristics make this technology a promising option to integrate reaction and separation processes into a single, compact unit for NH_3 synthesis. In this work, we aim to develop a novel MR for the in-situ removal of NH_3 by integrating new NH_3-selective carbon membranes (CMSM) within 3D printed Periodic Open Cellular Structures (POCS). Specifically, a base Python code is used to develop a 2D non-isothermal mathematical model of a membrane reactor, which is used to explore reactor performance at different operating conditions, to provide guidelines for the design stage and eventual scale-up. The reactor and permeation models were validated using kinetic experiments from the literature (Rossetti et al. [4]) and experimental tests conducted at lab scale, respectively. Subsequently, optimal operational conditions for a specific geometry (D=0.033 m, L=1.05 m) were found to be : [TR= 683K, TP=550K, PR=30 bar, PP=1 bar, GHSV=150 1/h, SW=0.2, y0 R=[H_2=0.573,N_2=0.382,NH_3=0.045]. These conditions yielded an NH_3 productivity of 63 g/h and a permeate stream purity of 20.6% resulting in an increase of 40% respect to the equilibrium conversion. Interesting was also the investigation of geometry effect in terms of reactor length and diameter, and distance between membranes. The DaPe number analysis revealed that longer reactors tend to favor NH_3 build- up at the top, while increasing the length of a reactor positively impacts the production capacity and purity. However, longer reactors require more catalyst, suggesting that the use multiple shorter reactors might be a better alternative.

Acknowledgment
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References
[1] Kaveh Mazloomi , et al., Renewable and Sustainable Energy Reviews 16, 2012
[2] Muhammad Aziz et al., Energies, 2020
[3] Enrico Drioli, Efrem Curcio, Journal of Chemical Technology and Biotechnology, 2007
[4] Ilenia Rossetti et al., Ind. Eng. Chem. Res, 2006

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Title: **[PP53]** Numerical Investigation of bubble size effect on the gas hold-up in a constant gas flow rate

Abstract: Bubble Columns are widely used in chemical engineering for various process applications. These applications take advantage of the ease of construction, flexibility in residence time, and good heat and mass transfer. Despite the simple construction, the hydrodynamics in bubble columns is complex, and a careful design (i.e., the column diameter, aspect ratio, and gas sparger openings) is necessary. The design of the gas sparger influences the gas hold-up, resident time, and liquid velocity. Bai et al. [1] reported that increasing the number of holes (perforated area) decreases the gas hold-up and liquid velocity. According to this research, the location of the sparger area affects both gas hold-up and bubble residence time. A deviation of the sparger from the center increases the resident time and intensifies the mixing rate. The experimental research of Besgani et al. [2] on sparger design showed that fine and coarse gas sparger produce a mono-dispersed and poly-dispersed homogenous respectively. In addition to the flow structure, the gas hold-up is highly dependent on the sparger hole size.

Despite the research on gas distribution inlets, there are questions to be addressed. For instance, (i), the effect of bubble size on gas hold-up and bubble residence time under a constant gas flowrate. (ii), the effect of the gas flow rate on turbulent kinetic energy and liquid velocity under a constant gas flowrate. (iii), changes in the gas hold-up as a function of superficial velocity.

In this research, Euler-Lagrange method is applied to solve a bubbly flow in a bubble column (air-water system). The numerical simulations in this research are performed using the in-house code “FoxBerry”[3]. A square bubble column with a size of 0.15m×0.15m, and a height of 0.45m is the modeling geometry. The collision of bubbles has been modeled with the Hard-sphere approach. The turbulence effect has been implemented using Large-Eddy Simulation. The optimum design is found to maximize the gas hold-up with the high kinetic energy rate. This design boosts the transport rate in a controlled way.

References

[1] Bai, W., Deen, N. G., & Kuipers, J. A. M. (2011). Industrial & Engineering Chemistry Research, 50(8), 4320-4328.

[2] Besagni, G., Gallazzini, L., & Inzoli, F. (2018). Chemical Engineering Science, 176, 116-126.

[3] Kamath, S., Masterov, M. V., Padding, J. T., Buist, K. A., Baltussen, M. W., & Kuipers, J. A. M. (2020). Journal of Computational Physics: X, 8, 100058.

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Title: **[PP54]** Eulerian-Lagrangian Simulation of Bubble-Liquid Interphase Mass Transfer in a Slurry Bubble Column

Abstract: Slurry bubble column reactors are encountered frequently in chemical and petrochemical industries. These reactors offer several advantages over other gas-liquid-solid reactors, including but not limited to enhanced rates of mass and heat transfer (Kantarci, Borak, 2005). An accurate prediction of their operation is required to improve their performance or design new reactors. However, the complexities originating from different transport phenomena accompanied by heterogeneous reactions make this a challenging task.

This study employs a Eulerian-Lagrangian approach to simulate a lab-scale slurry bubble column reactor, focusing on the interphase mass transfer between the bubbles and the slurry. This serves as a foundational step towards a comprehensive simulation that includes heat transfer and heterogeneous reactions.

The Lagrangian equation of motion is considered and solved for the gas bubbles, where the hydrodynamic forces exerted by the continuous phase are included in this equation, and each of the forces is calculated by a suitable model for the system (Tomiyama et al., 2002, Roghair et al., 2011). Moreover, the collision of the objects is accounted for by employing a soft- sphere approach. In the continuous phase, the volume-averaged Navier-Stokes equation is numerically solved, while the continuity equation is imposed using a projection method algorithm. To study the multi-component system, the species transfer equation for the continuous phase is considered with a source term to account for interphase mass transfer (Nedeltchev, 2017), and a Fickian diffusion model. A sub-grid scale model will be employed to include the effects of unresolved turbulent structures. The models are implemented in our in-house code, FoxBerry, which is responsible for the solution of conservation equations in all of the phases and coupling the Eulerian and the Lagrangian frameworks.

In this study, the effect of different solid particle loading in the reactor and as a consequence, the density and viscosity of the slurry phase on the mass transfer efficiency of the column will be investigated.

References

[1] N. Kantarci, F. Borak, Bubble column reactors, Process Biochemistry, 40, 2263-2283 (2005).

[2] A. Tomiyama, H. Tamai, I. Zun, S. Hosokawa, Transverse migration of single bubbles in simple shear flows, Chemical Engineering Science, 57, 1849-1858 (2002).

[3] I. Roghair, et al., On the drag force of bubbles in bubble swarms at intermediate and high Reynolds numbers, Chemical Engineering Science, 66, 3204-3211 (2011).

[4] S. Nedeltchev, Theoretical prediction of mass transfer coefficients in both gas–liquid and slurry bubble columns, Chemical Engineering Science, 157, 169-181 (2017).

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Title: **[PP55]** Development and Validation of an In-House CFD Code for Slurry Bubble Columns

Abstract: The slurry bubble column is a three-phase reactor with a continuous liquid phase seeded with particles that often have a catalytic function. The gas is injected into the column from the bottom through a sparger plate. The gas injection provides the column with reactants and aeration, it also enhances the mixing in the reactor. Slurry bubble columns are used in chemical and petrochemical industries, one such example is the production of synthetic fuels via the Fischer-Tropsch reaction. The FoxBerry in-house code, which employs the Eulerian-Lagrangian approach, is a multiphase CFD tool designed to simulate large-scale slurry bubble columns.

This study will use an Eulerian-Lagrangian framework to model the complex interactions within the slurry bubble column. The bubbles and the particles will be treated as the discrete phase and the continuous phase as the liquid. This multiphase flow simulation includes heat and mass transfer between the two different discrete phases and the discrete and continuous phases.

The in-house code will first be validated through a qualitative and quantitative comparison of the code with established Euler-Euler simulations of a two-phase bubble column. Deen et al[1] have performed an Eulerian-Eulerian simulation for the two-phase bubble column, capturing the essential hydrodynamics, including bubble-bubble interaction, and the induced turbulence of the bubbles.

All relevant hydrodynamic forces in the Deen case, including drag, virtual mass, lift, and wall forces will be considered. These forces will be applied to the discrete phase and various closure models for each hydrodynamic force will be analyzed. Turbulence will be modeled using the LES-SGS approach.

Since the original Deen case is the Eulerian-Eulerian approach the interactions between the bubbles are not considered. However, in this study, bubble-bubble interactions are crucial, since they influence the flow characteristics significantly. In this CFD-DEM approach, both the hard-sphere and soft-sphere models will be tested and compared.

The cross-sectional average fluid velocity will be used as a comparison parameter. The total simulated time of the bubble column is kept up to 150 seconds so that the statistical fluctuations are reduced for time averaging.

Once the in-house code is well-validated, the study will be expanded to include a large-scale two-phase bubble column and a three-phase slurry bubble column. Heat and mass transfer will be included in the later stage of the project.

References

[1] Deen, N. G., Solberg, T., & Hjertager, B. H. (2001). Large eddy simulation of the gas–liquid flow in a square cross-sectioned bubble column. Chemical engineering science, 56(21-22), 6341-6349.

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Title: **[PP56]** A Simplified Analytical Model for the Impurity Heating Hypothesis of Laser-Induced Crystal Nucleation

Abstract: One of the promising new crystallisation phenomena is called Non-Photochemical Laser-Induced Nucleation (NPLIN)[1]. In NPLIN experiments, irradiating supersaturated solutions with laser light may result in spontaneous nucleation of samples that would otherwise take weeks to crystallise. The susceptibility of a given chemical system to NPLIN is known to vary between chemical systems. For example, it is widely reported that the KCl- H_2O system undergoes NPLIN[1], but there is considerable evidence that the $NaClO_3$-H_2O system does not[2]. A successful theory of NPLIN should be capable of predicting whether a given supersaturated system is susceptible to NPLIN or not. One theory of NPLIN that has received significant attention in recent years is the Impurity Heating (IH) mechanism. This theory suggests that impurities are present in the solution, and that these absorb laser energy, causing them to heat up. The heated impurities in turn create hot spots and cause local evaporation, effectively acting as a kind of evaporative crystalliser. Despite recent numerical implementations of this mechanism[3,4], there is currently no easy way of evaluating the NPLIN susceptibility a priori. In this research, a simplified mathematical model of the IH mechanism is presented. The expected advantages are the reduction of the number of independent input parameters, and the overall ease of using the model for experimental design. The simplified mathematical model is derived from underlying partial differential equations by scaling analysis, and the resulting equations are compared with both previous computational models and experimental observations in the literature. The resulting model accurately fits to previous computational work on the concentration profile, but fits poorly with the expected temperature profile from the same simulations. The observation that the KCl-H_2O system is susceptible to NPLIN, and that the $NaClO_3$-H_2O system is not, are both reproduced. However, the model yields only very weak enhancement of nucleation rate in the case of $CO(NH_2)_2$, despite a large basis of experimental evidence to the contrary[1]. The latter observation can be interpreted as a limitation of the model due to oversimplification. Future research directions may include a more careful derivation going further than scaling analysis and a comparison with experimental evidence from other chemical systems.

References

[1] V. Korede, et al. Crystal Growth & Design, 23(5), 3873-3916.
[2] Barber, E. R. Non-photochemical laser-induced nucleation (NPLIN): an experimental investigation via real-time imaging and product analysis.
[3] N. Hidman, et al. Crystal Growth & Design, 20(11), 7276-7290
[4] N. Nagalingam, et al. Physical review letters, 131(12), 124001

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Title: **[PP57]** Energy and Exergy Analysis of a Coupled Dark Fermentation and Microbial Electrolysis Process for Sustainable Hydrogen Production

Abstract: This study simulates the coupling of dark fermentation and microbial electrolysis cells (MECs) to optimize biohydrogen production from vinasse, a byproduct of ethanol production, and glycerol, a byproduct of biodiesel production [1][2]. Dark fermentation breaks down organic substrates into hydrogen and volatile fatty acids [1][3], while MECs convert these byproducts into additional hydrogen with a small electrical input [2][3]. The coupling of these technologies enhances hydrogen yields and improves substrate utilization [2][3].

The simulation focuses on optimizing substrate concentration and operating conditions for co-processing vinasse and glycerol [1]. Vinasse serves as an abundant substrate for microbial activity [4][5], while glycerol provides an additional carbon source. Coupling dark fermentation with MECs further boosts hydrogen recovery, utilizing residual compounds from fermentation [2][3].

Energy and exergy analyses were conducted to assess system performance, providing a comprehensive understanding of how different factors impact the efficiency of the coupled process [1] [4]. A Monte Carlo simulation analyzed the influence of glycerol composition on energy and exergy performance, offering insights into process variability and robustness under a range of conditions [1]. The energy analysis revealed MECs achieve up to 91% hydrogen capture, though challenges like scaling and low reaction yields reduce overall efficiency. Exergy analysis identified areas for energy recovery, highlighting the potential for improved system efficiency by minimizing irreversibility and optimizing energy utilization within the process [4].

Despite these promising results, scalability and operation present challenges [1]. However, this coupled system shows potential for advancing waste-to-energy technologies and supporting the circular economy through sustainable biohydrogen production from industrial waste streams [2].

References

[1] R. Gong and B. H. Lunelli, "Exergy Analysis of Biogas Production from Sugarcane Vinasse".
[2] P. Srivastava, et al. "Coupling dark fermentation and microbial electrolysis cells for higher hydrogen yield: Technological competitiveness and challenges".
[3] Y. Lo, et al. "Dark fermentative hydrogen production with crude glycerol from biodiesel industry using indigenous hydrogen-producing bacteria".
[4] E. Carrilho, et al. "DESTINATION OF VINASSE, A RESIDUE FROM ALCOHOL INDUSTRY: RESOURCE RECOVERY AND PREVENTION OF POLLUTION".
[5] R. Haron, et al. "Conversion of crude glycerol to biohydrogen by locally isolated Klebsiella pneumoniae via dark fermentation".

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Title: **[PP58]** Design of a separation system for the closed-loop superheated steam drying process in the paper industry

Abstract: We live in an era where we must drastically reduce our greenhouse gas emissions. Most of these emissions are the result of our need for energy. Our industries require vast amounts of energy. The European Union's top 3 industries with the highest energy consumption in 2022 were the chemical and petrochemical, non-metallic and paper, pulp, and printing industries [1]. In a paper-making process, the paper drying step accounts for 70% of the energy requirements, i.e., there is scope for improvement [2]. Superheated steam drying (SHSD) is a promising drying method, potentially reducing the energy requirements by 70% and related CO_2 emissions by 88% compared to air drying with drying cylinders and steam from natural gas combustion [2]. As the paper is dried in the SHSD, the steam is contaminated with dust and non-condensable. These contaminants can cause operational issues and reduce the efficiency of the drying process. Therefore, the contaminants must be effectively controlled to maintain a closed-loop process.

Based on this potential, the European Steam Dry project commenced beginning of 2024 to explore the application of superheated steam drying in the paper industry. The role of the University of Twente is to ensure high-quality steam in the closed-loop SHSD process by executing a model-based separation system design for recovering the steam. It is expected that a model-based approach will improve the performance of the equipment and reduce the energy consumption and the costs.

Our approach begins with a comprehensive review of existing separation methods and to understand the steam's characteristics that need to be treated. From this review, a suitable separation technology can be identified. Once the technology is selected, a dynamic model is developed to describe the separation performance as a function of time and operational variables. The model will be validated and verified with experimental data. Once the model is validated, it can be used to set up an optimization and control strategy, to find the best settings for the separation equipment. The optimization can be a challenging task, as it is expected that the performance of the separation equipment over time will deteriorate and cleaning of the equipment is needed. For this reason, the model needs a scheduler, that can alternate between separation mode and cleaning mode. Model and scheduler will be used to create a digital twin that can be accessed and used by different stakeholders.

References

[1] Eurostat: Final energy consumption in industry. [Accessed on 2024-07-05]
[2] Wilk, V., Knöttner, S. B., Drexler-Schmid, G., & Barz, T. (2023). Superheated steam drying for paper production: process efficiency assessment. https://doi.org/10.52202/069564-0128

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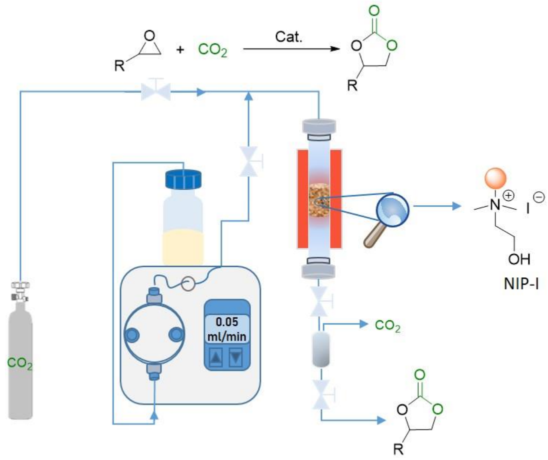
Title: **[PP59]** Resin beads as metal-free catalysts for the synthesis of cyclic carbonates

Abstract: Using CO_2 as a C1 feedstock for the synthesis of value-added chemicals has been extensively studied in recent years due to its green characteristics, such as being clean, abundant, and renewable.[1] One promising method of CO_2 utilisation is its atom-economical conversion with epoxides into cyclic carbonates (estimated market size: 100 ktonnes per year in 2013). The synthesis of cyclic carbonates via the cycloaddition of CO_2 to epoxides is typically carried out in batch reactors, with the catalyst recovered through filtration or distillation after the reaction.[2] Alternatively, using a fixed-bed reactor allows for continuous operation, avoiding the additional catalyst separation step, which is preferable for industrial applications. However, limited examples have demonstrated the synthesis of cyclic carbonates through CO_2 cycloaddition to epoxides in a fixed-bed reactor.[3, 4]



To identify an efficient catalyst for the continuous synthesis of styrene carbonates in a fixed-bed reactor, we began by screening fifteen commercially available resin beads containing I^- (after ion exchange with KI) in a high-throughput batch reactor. These resin beads vary in their polymer backbone, porosity (e.g. gel/porous), and functional groups (e.g. -OH). The screening tests revealed that resin beads with a porous structure and functionalised with a -OH group generally outperformed the other selected resin beads. Further studies showed that grinding these resin beads into powder enhanced the accessibility of active sites within the polymer matrix. This approach significantly benefited the gel-type resin beads, which exhibited a maximum of nine times higher catalytic activity than the counterpart beads catalyst. Among them, the NIP-I powder catalyst showed the highest catalytic activity (84% yield, TON 104), prompting further studies in the fixed-bed reactor using the N-IP-I catalyst. Under the optimised reaction conditions, NIP-I catalyst showed a steady and high styrene carbonate yield (62% yield on average, productivity 5.3 h^{-1}) over the tested a time-on-stream of 12 h.

References

1. *Nature*, 2019, **575**, 87-97.
2. *Green Chemistry*, 2019, **21**, 406-448.
3. *RSC Advances*, 2017, **7**, 2836-2841.
4. *Applied Catalysis A: General*, 2016, **519**, 146-154.

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