NPS2023

Netherlands Process technology Symposium

Engineering a Better Tomorrow

6 & 7 July 2023

Book of Abstracts

UNIVERSITY
OF TWENTE.

Kinepolis | Colosseum 60 | Enschede | nps2023@utwente.nl

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Word of Welcome

We hope you enjoy this book of abstracts for the 18th edition of the Netherlands Process technology Symposium to be held in Kinepolis, Enschede from 6-7 July 2023.

NPS2023 is the leading event to stay on top of advancements in process engineering, and provides opportunities to meet with colleagues from academia and industry. Process engineering is more important than ever, taking a key role in developing solutions for numerous societal challenges and the energy transition. We want to highlight academic research in sustainable process technology, and connect it with the needs from society and industry.

Meik, Edwin, Aayan, Marie,
Jimmy, Anne

We would like to thank our sponsors for supporting NPS2023

HoST BIOENERGY SYSTEMS

DEMCON | SUSTER

UNIVERSITY OF TWENTE.
Faculty of Science of Technology

AVEBE

NPT Nederlandse Procestechnologen

Timetable

6th of July

Time	Room			
	Room 6	Room 7	Room 8	Room 5
08:30 - 09:00	**Registration** ***(Foyer Kinepolis)***			
09:00 - 10:45	**Opening, Welcome and Plenary I & II** ***(Room 5)***			
10:45 - 11:15	**Coffee Break** ***(2nd floor Kinepolis)***			
11:15 - 12:30	**Parallel 1.1** **Bioprocess Engineering, Food & Pharma** ***(incl. Keynote 1)***	**Parallel 1.2** **Circularity & Sustainability** ***(incl. Keynote 2)***	**Parallel 1.3** **Electrochemical Engineering**	**Parallel 1.4** **Reactor Engineering & Transport Phenomena**
12:30 - 13:30	**Lunch Break** ***(2nd floor Kinepolis)***			
13:30 - 14:45	**Parallel 2.1** **Process Systems Engineering** ***(incl. Keynote 3)***	**Parallel 2.2** **Bioprocess Engineering, Food & Pharma** ***(incl. Keynote 4)***	**Parallel 2.3** **Seperation Technology & Thermodynamics**	**Parallel 2.4** **Reactor Engineering & Transport Phenomena**
14:45 - 15:15	**Coffee Break** ***(2nd floor Kinepolis)***			
15:15 - 16:30	**Plenary III + Poster Parade** **(room 5)**			
16:30 - 18:00	**Poster session & welcome reception** ***(2nd floor Kinepolis)***			
19:00 - 21:00	**Conference dinner** **(Fletcher Hotel, De Bakspieker)**			

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7th of July

Time	Room			
	Room 6	Room 7	Room 8	Room 5
08:30 - 09:00	**Registration** ***(Foyer Kinepolis)***			
09:00 - 10:45	**Announcements, Plenary IV, and Poster Parade** ***(Room 5)***			
10:45 - 11:15	**Coffee break** ***(2nd floor Kinepolis)***			
11:15 - 12:30	**Parallel 3.1** **Circularity & Sustainability**	**Parallel 3.2** **Seperation Technology & Thermodynamics**	**Parallel 3.3** **Electrochemical Engineering**	**Parallel 3.4** **Reactor Engineering & Transport Phenomena**
12:30 - 13:30	**Poster Session + Lunch Break** ***(2nd floor Kinepolis)***			
13:30 - 14:45	**Parallel 4.1** **Circularity & Sustainability** ***(incl. Keynote 5)***	**Parallel 4.2** **Process Systems Engineering** ***(incl. Keynote 6)***	**Parallel 4.3** **Separation Technology & Thermodynamics**	**Parallel 4.4** **Reactor Engineering & Transport Phenomena**
14:45 - 15:15	**Coffee Break** ***(2nd floor Kinepolis)***			
15:15 - 16:15	**Plenary V, Awards and Closing Ceremony** ***(Room 5)***			

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Themes

During NPS 2023 we have six themes that encompass our motto ‘Engineering a Better Tomorrow’. These are:

- ◊ Reaction Engineering & Transport Phenomena
- ◊ Electrochemical Engineering
- ◊ Seperation Technology & Thermodynamics
- ◊ Bioprocess Engineering, Food & Pharma
- ◊ Process Systems Engineering & Industry 4.0
- ◊ Circularity & Sustainability

Instructions for presenters

Please contact the chair of your session 15 minutes prior to the start of your parallel session and make sure you upload and test the presentation. You can also upload your presentation before the start of NPS2023 here.

For posters, please upload your poster 4th of July at the latest here, so we can prepare for the poster parade.

Plenary
Timing: 40 minutes presetation + 5 minutes discussion

Keynote
Timing: 25 minutes presentation + 5 minutes discussion

Oral
Timing: 12 minutes presentation + 3 minutes discussion

Poster
A0 Poster + 3 slides for the poster parade (pitch presentation of 2 minutes)

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Scientific Committee

We want to thank the scientific committee for taking the time to read and rate all the abstracts submitted for NPS 2023. Without them it would have been impossible to have this symposium.
In no specific order:

- Artur Schweidtmann
- Jeroen Jansen
- Remko Boom
- Karin Schroen
- Sascha Kersten
- Antoni Forner Cuenca
- Bastian Mei
- Guido Mul
- David Fernandez
- Fausto Galluci
- Hans Kuipers
- Vasilis Kyriakou
- John van der Schaaf
- Zandri Borneman
- André de Haan
- Antoine Kemperman
- Boelo Schuur

Program Oral Presentations

5th & 6th of July

Wednesday 5th of July 2023

NPS Business Dinner (by invitation only)

From 19:00 to 22:00, U Parkhotel (Board room, 9th floor)

Thursday 6th of July 2023

Registration

From 08:30 to 09:00, Kinepolis (Foyer, Main Entrance)

Welcome and Plenary lecture I & II

From 09:00 to 10:45, Kinepolis (Room 5)

Chaired by: Meik Franke & Edwin Zondervan

9:30 **[Plen01] Title:** (Bio)waste for Tomorrow's Chemicals
Presenter: Herman Klein Teeselink (HoST)

10:15 **[Plen02] Title:** Digital Transformations of Chemical Engineering Science
Presenter: Hans Hasse (RPTU, Rheinland-Pfälzische Technische Universität Kaiserlautern-Landau)

Coffee Break

From 10:45 to 11:15 to 12:30, Kinepolis (2nd Floor)

Parallel Session 1.1 Bioprocess Engineering, Food & Pharma

From 11:15 to 12:30, Kinepolis (Room 6)

Chaired by: Karin Schroen

11:15 **[K01] Title (Keynote Lecture):** Efficient pretreatment of lignocellulosic biomass with hot liquid water for co-product valorization
Presenter: Adrie Straathof (Delft University of Technology)

11:45 **[L01] Title:** Liquid-liquid extraction of medical radioisotopes in microfluidic channels treated by atomic layer
Presenter: Albert Santoso (Delft University of Technology)

12:00 **[L02] Title:** A plant wide simulation of polyhydroxyalkanoate production from waste water and its conversion to methyl crotonate
Presenter: Akbar Asadi Tashvigh (Wageningen University & Research)

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12:15 **[L03] Title:** Coupling hydrodynamics and metabolic dynamics in syngas fermentation guiding industrial reactor design
Presenter: Lars Puiman (Delft University of Technology)

Parallel Session 1.2 Circularity & Sustainability

From 11:15 to 12:30, Kinepolis (Room 7)

Chaired by: Sascha Kersten

11:15 **[L04] Title:** Eco- friendly recovery of valuable by-products for enhancing hot-liquid water pretreatment of biomass
Presenter: Tamara Janković (Delft University of Technology)

11:30 **[L05] Title:** Industrial Production Of Propylene Using Dense Ceramic Membranes
Presenter: Jord Peter Haven (University of Twente)

11:45 **[L06] Title**: Modeling of syngas fermentation: a Gibbs free energy-constrained black-box model that predicts selectivity between ethanol and acetic acid
Presenter: Eduardo Francisco Almeida Benalcázar (Delft University of Technology)

12:00 **[K02] Title (Keynote Lecture):** Teaching break-through process concept design by functions
Presenter: Jan Harmsen (Harmsen Consultancy B.V.)

Parallel Session 1.3 Electrochemical Engineering

From 11:15 to 12:30, Kinepolis (Room 8)

Chaired by: Bastian Mei

11:15 **[L07] Title:** Design of an Elevated Pressure Electrochemical Flow Cell for \
CO2 Reduction
Presenter: Nandalal Girichandran (Delft University of Technology)

11:30 **[L08] Title:** Development of high differential pressure AEM electrolyzer
Presenter: Anirudh Venugopal (HyET E-Trol)

11:45 **[L09] Title:** Suspension electrodes for electrochemical CO2 reduction
Presenter: Nathalie E.G. Ligthart (Delft University of Technology)

12:00 **[L10] Title:** Clay composite membranes for salinity gradient batteries
Presenter: Nadia Boulif (Eindhoven University of Technology)

12:15 **[L11] Title:** Dendritic Iron Formation in Low-Temperature Iron Oxide Electroreduction Process using Alkaline Solution
Presenter: Akmal Irfan Majid (Eindhoven University of Technology)

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Parallel Session 1.4 Reactor Engineering & Transport Phenomena

From 11:15 to 12:30, Kinepolis (Room 5)

Chaired by: Martin van Sint Annaland

11:15 **[L12] Title:** The mechanism behind vibro-assisted fluidization of cohesive micro-silica
Presenter: Rens Kamphorst (Delft University of Technology)

11:30 **[L13] Title:** Stirrer design for improving fluidization of cohesive powders
Presenter: Kaiqiao Wu (Delft University of Technology)

11:45 **[L14] Title:** Understanding particle flows in sub-fluidized horizontal stirred bed reactors by radioactive particle tracking
Presenter: Pieter Christian van der Sande (Delft University of Technology)

12:00 **[L15] Title:** Hydrodynamic study of single- and two-phase flows in packed bed microreactors
Presenter: Lu Zhang (University of Groningen)

12:15 **[L16] Title:** Solidification and Solute Redistribution During a Progressive Freeze Concentration Process -Theoretical Modeling and Experimental Validation
Presenter: Sara Filipa Bentes Da Conceicao (Delft University of Technology)

Lunch

From 12:30 to 13:30, Kinepolis (2nd Floor)

Parallel Session 2.1 Process Systems Engineering

From 13:30 to 14:45, Kinepolis (Room 6)

Chaired by: Artur Schweidtmann

13:30 **[K03] Title (Keynote lecture):** Multiscale and multidisciplinary modelling for the sustainable design of co-electrolysis systems
Presenter: Mar Pérez-Fortes (Delft University of Technology)

14:00 **[L17] Title:** Fabricating multi-scale materials via in-air microfluidics
Presenter: Claas Willem Visser (University of Twente)

14:15 **[L18] Title:** Effect of gaseous contaminants on electrochemical CO2 reduction to C2+ products
Presenter: Asvin Sajeev Kumar (Delft University of Technology)

14:30 **[L19] Title:** Using a superstructure approach for techno-economic analysis of membrane processes
Presenter: Rouzbeh Ramezani (Eindhoven University of Technology)

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Parallel Session 2.2 Bioprocess Engineering, Food & Pharma

From 13:30 to 14:45, Kinepolis (Room 7)

Chaired by: Adrie Straathof

13:30	**L20] Title:** Membrane performance and mass transfer with adjusting solution pH and ionic strength during fractionating a fish protein hydrolysate **Presenter**: Nattawan Chorhirankul (Wageningen University & Research)
13:45	**[L21] Title:** Dry fractionation for sustainable recovery of protein enriched ingredients: A focus on powder properties **Presenter** : Regina Politiek (Delft University of Technology)
14:00	**[L22] Title:** Prediction of Permeate Flux and Rejection during Microfiltration of Skim Milk at Low Temperature Using a Geometric Model **Presenter** Hilda Lucy Nyambura (Wageningen University & Research)
14:15	**[K04] Title (Keynote lecture):** Technology: a crucial component in food transition. How a Dutch cooperative contributes to more sustainable foods **Presenter**: Kees Maarschalk (Avebe)

Parallel Session 2.3 Separation Technology & Thermodynamics

From 13:30 to 14:45, Kinepolis (Room 8)

Chaired by: Arian Nijmeijer

13:30	**[L23] Title:** Understanding Ion Crossover in Acid-Base Flow Battery for Long Duration Energy Storage **Presenter**: Kaustub Singh (Delft University of Technology)
13:45	**[L24] Title:** Dynamic ammonium retention in membrane processes for nutrient separation from manure **Presenter**: Marrit van der Wal (Eindhoven University of Technology)
14:00	**[L25] Title:** Study of organic solvents in the extraction of lignin and furanics from deep eutectic **Presenter**: Mahsa Gholami (University of Twente)
14:15	**[L26] Title:** Laser-Induced Cavitation for Controlling Crystallization from Solution **Presenter**: Burak Eral (Delft University of Technology)
14:30	**[L27] Title:** Reactive extraction-promoted 5-hydroxymethylfurfural production in deep eutectic solvents in batch reactors and microreactors **Presenter**: Chencong Ruan (University of Groningen)

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Parallel Session 2.4 Reactor Engineering & Transport Phenomena

From 13:30 to 14:45, Kinepolis (Room 5)

Chaired by: Name

13:30 **[L28] Title:** LOGIC 2.0: Towards a natural convection driven, autothermal and condensing methanol reactor
Presenter: Tim van Schagen (University of Twente)

13:45 **[L29] Title:** Catalyst deactivation in methanol synthesis
Presenter: Lola Azancot Luque (University of Twente)

14:00 **[L30] Title:** Experimental study of droplet-side mass transfer in slug flow capillary microreactors
Presenter: Tingting Wang (University of Groningen)

14:15 **[L31] Title**: Numerical investigation of the primary break-up of a jet for laminar and turbulent conditions
Presenter: Cristina García Llamas (Eindhoven University of Technology)

14:30 **[L32] Title:** Photochemical Transformations using the Rotor-Stator Spinning Disc Reactor
Presenter: Arnab Chaudhuri (Delft University of Technology)

Coffee Break

From 14:45 to 15:15, Kinepolis (2nd Floor)

Plenary lecture III & Poster Parade

From 15:15 to 16:30, Kinepolis (Room 5)

Chaired by: Jimmy Faria Albanese & Anne Tiehuis

15:15 **[Plen03] Title:** Chemical Recycling of Packaging Plastic Waste via Thermal Pyrolysis
Presenter: Pilar Ruiz Ramiro (University of Twente)

16:00 15 relay poster presentations (each 2 minutes)

NPS Reception

From 16:30 to 18:00, Kinepolis (2nd Floor)

Conference Dinner

From 19:00 to 22:00, Fletcher Hotel De Broeierd (De Bakspeieker)

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7th of July

Friday 7th of July 2023

Registration

From 08:30 to 09:00, Kinepolis (Foyer, Main Entrance)

Excursion Microfarm Biogas Plant (HoST) (by registration)

From 09:00 to 12:00, Deurningen

Plant excursion for students offered by HoST, pick-up from Kinepolis

Announcements, Plenary IV & Poster Parade

From 09:00 to 10:45, Kinepolis (Room 5)

Chaired by: Marie-Alix Pizzocarro & Anne Tiehuis

09:20 **[Plen04]** Defosilizing the industrial sector: from incrementalism to radical disruption
Presenter: Andrea Ramirez (Delft University of Technology)

10:05 26 Relay poster presentations (each 2 minutes)

Coffee Break

From 10:45 to 11:15, Kinepolis (2nd Floor)

Parallel Session 3.1 Circularity & Sustainability

From 11:15 to 12:30, Kinepolis (Room 6)

Chaired by: Andrea Ramirez

11:15 **[L33] Title:** Stability of potassium-promoted hydrotalcite for CO2 capture under different adsorption/desorption cycles
Presenter: Kun Xin (Eindhoven University of Technology)

11:30 **[L34] Title:** Chemical recycling of plastic waste: from polyolefins to short alkanes via hydrogenolysis
Presenter: Eline van Daatselaar (University of Twente)

11:45 **[L35] Title:** Cellulase enzyme recovery from cellulosic hydrolysate
Presenter: Elchin Jafariyeh Yazdi (University of Groningen)

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12:00 **[L36] Title:** Exploring the Intrinsic Kinetics of Polyolefins Pyrolysis in a Screen Heater Reactor
Presenter: Dwiputra Muhammad Zairin (University of Twente)

12:15 **[L37] Title**: Chemical Recycling of Polyurethanes: Conversion of Carbamates
Presenter: Shahab Zamani Gharaghooshi (University of Twente)

Parallel Session 3.2 Separation Technology & Thermodynamics

From 11:15 to 12:30, Kinepolis (Room 7)

Chaired by: Zandri Borneman

11:15 **[L38] Title**: Growth dynamics of aspirin crystals in microfluidic antisolvent crystallization
Presenter: Vikram Korede (Delft University of Technology)

11:30 **[L39] Title:** Supercritical Drying Of Starch
Presenter: Federico Perondi (University of Groningen)

11:45 **[L40] Title:** Layer-by-layer modified electrospun bipolar membranes for enhanced water dissociation
Presenter: Menno Houben (Eindhoven University of Technology)

12:00 **[L41] Title:** Electrochemically mediated carbon monoxide separation
Presenter: Christel Koopman (Delft University of Technology)

12:15 **[L42] Title:** Carbon Molecular Sieve Membranes for separation of Helium from Natural Gas
Presenter: Arash Rahimalimamaghani (Eindhoven University of Technology)

Parallel Session 3.3 Electrochemical Engineering

From 11:15 to 12:30, Kinepolis (Room 8)

Chaired by: Guido Mul

11:15 **[L43] Title:** OH- selective thin film composite membranes can prevent CO2 loss in CO2 electrolysis
Presenter: Kostadin Veselinov Petrov (Delft University of Technology)

11:30 **[L44] Title:** Engineering gas diffusion electrode microstructures for the electrochemical reduction of CO2 to ethylene
Presenter: Senan F. Amireh (Eindhoven University of Technology)

11:45 **[L45] Title:** Thermal implications in next-generation CO2 electrolyzers: a hot topic
Presenter: Jan-Willem Hurkmans (Delft University of Technology)

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12:00 **[L46] Title:** Anion exchange membranes for the electrochemical reduction of C)2
Presenter: Woutje ter Weel (Eindhoven University of Technology)

12:15 **[L47] Title**: Modeling optimal operational strategies for alkaline electrolyser under dynamic power input conditions
Presenter: Michele Tedesco (TNO)

Parallel Session 3.4 Reactor Engineering & Transport Phenomena

From 11:15 to 12:30, Kinepolis (Room 5)

Chaired by: John Padding

11:15 **[L48] Title:** Visualizing pH and mass transport in electrolyser with new FLIM probes
Presenter: Jorrit Bleeker (Delft University of Technology)

11:30 **[L49] Title:** 3D Air Bubble Shape Reconstruction from 2D Imagery using Neural Net works and Spherical Harmonics
Presenter: Douwe Orij (Eindhoven University of Technology)

11:45 **[L50] Title:** Predicting the steady-state performance of Pickering emulsion reactors
Presenter: Valeria Garbin (Delft University of Technology)

12:00 **[L51] Title**: Study of the Hydrodynamics in a Trickle Bed Reactor using Particle-resolved Simulations
Presenter: Arvin Tavanaei (Eindhoven University of Technology)

12:15 **[L52] Title:** Development of long-term Hydrogen storage technologies through green ammonia production in innovative Catalytic Membrane Reactor (CMR)
Presenter: Iolanda Gargiulo (Eindhoven University of Technology)

Lunch & Poster Session

From 12:30 to 13:30, Kinepolis (2nd Floor)

Parallel Session 4.1 Circularity & Sustainability

From 13:30 to 14:45, Kinepolis (Room 6)

Chaired by: Mar Pérez-Fortes

13:30 **[K05] Title:** Python in Chemical Process Simulation
Presenter: Armin Fricke (CGC Capital-Gain Consultants GmbH)

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13:45 **[L53] Title :** Unravelling the impact of using alternative carbon feedstocks in existing petrochemical clusters
Presenter: Andrea Ramirez (Delft University of Technology)

14:00 **[L54] Title:** Wind Turbine Blade Recycling Process Which Fits the Circular Economy System Concept
Presenter: Maximiliano Taube (Delft University of Technology)

14:15 **[L55] Title:** Production of 1,2-propanediol by the aqueous phase hydrogenolysis of glycerol without external hydrogen addition over Ni/Al3Fe1: effect of the calcination temperature
Presenter: Raquel Raso Roka (Universidad de Zaragoza)

Parallel Session 4.2 Process Systems Engineering

From 13:30 to 14:45, Kinepolis (Room 7)

Chaired by: Tony Kiss

13:30 **[L56] Title:** Optimal scheduling and sizing for a microbial electrosynthesis plant integrated with renewable electricity
Presenter: Jisiwei Luo (Delft University of Technology)

13:45 **[L57] Title:** Physics-informed reinforcement learning for process design
Presenter: Ernst Uijthof (University of Twente)

14:00 **[L58] Title:** Optimization of a Membrane Cascade for Binary Gas Separation under Uncertainty of Membrane Properties
Presenter: Albertus Fuad Prajna Harto Subagyo (University of Twente)

14:15 **[K06] Title (Keynote lecture):** Designing Chemical Manufacturing Automation with Care
Presenter: Michael Wartmann (Nouryon Chemicals B.V.)

Parallel Session 4.3 Separation Technology & Thermodynamics

From 13:30 to 14:45, Kinepolis (Room 8)

Chaired by: Boelo Schuur

13:30 **[L59] Title:** Comparison of solvent and sorbent-based carbon capture systems in LNG-fueled ships
Presenter: Jayaram Ganesan (University of Twente)

13:45 **[L60] Title:** Process synthesis and design of intensified distillation sequences
Presenter: Qing Li (Delft University of Technology)

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14:00 **[L61] Title:** Purification of CO2-based lactic and glyoxylic acids using membrane technology
Presenter: Paulina A. Sosa Fernandez (University of Twente)

14:15 **[L62] Title:** A hybrid hollow fiber nanofiltration process for organic micro-pollutant removal from wastewater
Presenter: Hans David Wendt (University of Twente)

14:30 **[L63] Title:** Evaporative crystallization of sessile droplets using electrowetting
Presenter: Qi An (Delft University of Technology)

Parallel Session 4.4 Reactor Engineering & Transport Phenomena

From 13:30 to 14:45, Kinepolis (Room 5)

Chaired by: Wim Brilman

13:30 **[L64] Title:** Operando spatial reactor analysis for the kinetic study of oxidative coupling of methane
Presenter: Jose Palomo Jimenez (Delft University of Technology)

13:45 **[L65] Title:** Precipitation of species during drying in catalyst preparation
Presenter: D.R. (David) Rieder (Eindhoven University of Technology)

14:00 **[L66] Title:** Solidification and Solute Redistribution During a Progressive Freeze Concentration Process -Theoretical Modeling and Experimental Validation
Presenter: Zhuo Zhang (University of Twente)

14:15 **[L67] Title**: Sublimation temperature of carbon dioxide for varying ambient pressure and far-field concentration
Presenter: Abhishek Purandare (University of Twente)

14:30 **[L68] Title:** Ru-based nanocatalysts for ammonia production in Membrane Reactors
Presenter: Gaetano Anello (Eindhoven University of Technology)

Coffee Break

From 14:45 to 15:15, Kinepolis (2nd Floor)

Plenary Lecture V, Awards & Closing Ceremony

From 15:15 to 16:35, Kinepolis (Room 5)

Chaired by: Aayan Banerjee & Meik Franke

15:15 **[Plen05]** Accelerating Pathways to ‘Net-Zero’: Development of Electro(-chemical) Driven Reactors/Separators
Presenter: Peter Veenstra, (Shell)

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Program Poster Presentations

6th of July

Poster Parade

From 15:15 to 16:30, Kinepolis (Room 5)

15:15 **[P01] Title:** Designing Gas Diffusion Electrodes with Tailored Wettability for CO2 Reduction Electrolyzers
Presenter: Mert Can Erer

[P02] Title: The conversion of furfural to bio jet fuel
Presenter: Rick Baldenhofer

[P03] Title: Surface functionalization of Cu electrocatalysts for the electrochemical reduction of CO2 to ethylene with improved selectivity and durability
Presenter: Jesse Thomas Benjamin de Boer

[P04] Title: On the influence of trialkylamine reduction strategies in the direct hydrogenation of CO2 to formic acid
Presenter: Anouk de Leeuw den Bouter

[P05] Title: Heterogeneously SnPd-catalysed Nitrate and Nitrite reduction in aqueous solution
Presenter: Janek Betting

[P06] Title: Cobalt-based Fischer-Tropsch Synthesis catalysts for the conversion of CO2-rich syngas
Presenter: tba

[P07] Title: Creating lumped models for fluidized bed gasifiers using CFD
Presenter: Ravi Ramesh

[P08] Title: The Drive-Down System for Production, Storage, and Transport of Emission-Free Hydrogen
Presenter: Albertus Fuad Prajna Harto Subagyo

[P09] Title: Digitization of Process and Instrumentation Diagrams (P&IDs) using Deep Learning
Presenter: Artur Schweidtmann

[P10] Title: Liquid Organic Hydrogen Carriers - Process design and economic analysis for manufacturing N-ethylcarbazole
Presenter: Vivek Chandran Komath

[P11] Title: Verification of the Nanoparticle Heating Mechanism in Laser-Induced Nucleation of KCl Solution
Presenter: Pingping Cui

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[P12] Title: Micromixing efficiency in the turbulent boundary layers in a rotor-stator spinning disc reactor
Presenter: Christianus Hop

[P13] Title: Experimental studies on pressure drop and heat transfer in 3D printed baffled logpile structures
Presenter: Timothy van Lanen

[P14] Title: Integrating CO2 capture and electrochemical conversion using a bicarbonate flow cell: optimizing Cu/Ag foam electrode configuration for the production of ethylene and ethanol
Presenter: Iris Burgers

[P15] Title: Gas crossover in advanced zero-gap alkaline water electrolysis
Presenter: Rodrigo Lira Garcia Barros

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7th of July

Poster Parade

From 10:05 to 10:45, Kinepolis (Room 5)

[P16] Title: Surrogate models for the optimal design of distillation columns with vari able compositions
Presenter: Ana Somoza-Tornos

[P17] Title: Impact of varying macronutrient composition on 3D printability of pea-based food formulations
Presenter: Aaditya Venkatachalam

[P18] Title: Electrically driven non-thermal dewatering of biomass (ELECTRIFIED)
Presenter: Maarten Schutyser

[P19] Title: Dry fractionation for sustainable recovery of protein enriched ingredients: A focus on powder properties
Presenter: Regina Politiek

[P20] Title: Assessment of a bio-molecular sensor in the operation of adsorption processes-A model based approach
Presenter: Leyla Ozkan

[P21] Title: ARTIS
Presenter: Hans van de Vorst

[P22] Title: Tuning mesoporous ceramic membranes for solvent nanofiltration
Presenter: Daan Borger

[P23] Title: Selection of green organic entrainers and natural deep eutectic solvents (NADESs) for azeotrope/close-boiling mixture separation by extractive distillation
Presenter: Dhoni Hartanto

[P24] Title: Study on turbulent flow and droplets behavior to optimize coalescence filter separators
Presenter: Weiran Zhang

[P25] Title: Electro-responsive hydrogels for implementation in dewatering and deionizing processes
Presenter: Esli Diepenbroek

[P26] Title: Properties of polyhydroxyalkanoate membranes formed using non-halogenated solvents
Presenter: Liang-Shin Wang

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[P27] Title: Process development of enhanced furfural production via boronic acid intermediates
Presenter: Peter van der Wal

[P28] Title: Methane oxidation on Pd/CeO2 nanorods, nanocubes and octahedra at low temperatures; structure-dependent activity and poison resistance
Presenter: Martim Chiquetto Policano

[P29] Title: Engineering of two-dimensional nanomaterial layers acting as membranes and reactive electrochemical separation systems
Presenter: Famke Sprakel

[P30] Title: Recyclable Bio-Based Thermoplastic Materials from Liquefied Wood
Presenter: Sterre van der Voort

[P31] Title: Preparation of Electrospun Forward Osmosis Membranes for Clean Water Production
Presenter: Aylin Kinik

[P32] Title: Exploring the detrimental effect of water activity on liquid phase fatty nitrile production for in-situ water removal
Presenter: Carola Raffel

[P33] Title: The Infinity Reactor: A new conceptual design for a more cost-efficient CO2 to methanol route
Presenter: Hilbert Keestra

[P34] Title: THOR- Inductive Heating of Processes
Presenter: Soraya Sluijter

[P35] Title: Modeling and simulation of reverse water gas shift reaction with induction heating
Presenter: Liangyuan Wei

[P36] Title: A systems perspective on chemicals manufacturing via electrochemical reduction of CO2
Presenter: Riccardo Dal Mas

[P37] Title: Solvent screening for purification of technical cashew nut shell liquid using COSMO-based methods
Presenter: Isabella Arenas Bustos

[P38] Title: Coupling hydrodynamics and metabolic dynamics in syngas fermentation guiding industrial reactor design
Presenter: Romolo Di Sabatino

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Author: Herman Klein Tesselink (HoSt)

Title: **[PlenL01] (Bio)Waste for Tomorrow’s Chemicals**

Bio: Herman Klein Teeselink has a Master Chemical engineering (1985) and started to work at an engineering company. In 1986 he went to Stork to become a specialist in gasification CHP. In 1988 he gained his master Industrial Engineering & Management. In 1991 Stork and Holec asked him to set up a consultancy company on energy saving in the industry: HoSt. In 1999 he bought HoSt from the original owners and transformed the company to a mayor supplier of bioenergy systems like biogas units, biogas upgrading, biomass fired combined heat and power, CO2 capture from flue gasses CO2 liquification.

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Author: Hans Hasse (RPTU Kaiserlautern)

Title: **[Plen02] Digital Transformation of Chemical Engineering Science**

Bio: Prof. Hans Hasse is a Professor of Thermodynamics at RPTU Kaiserslautern, Germany. His research focusses on properties of complex fluid mixtures and links molecular thermodynamics to fluid separation process design. He is author of more than 400 scientific papers and 40 patents and has received many distinctions, including an ERC Advanced Grant and the Ernest Solvay Prize. Since 2020, he is Vice President of the German Science Foundation DFG. Before joining RPTU Kaiserslautern, he was a Professor of Thermodynamics and Fluid Separations at University of Stuttgart, and a process engineer at BASF, Ludwigshafen.

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Author: M. Pilar Ruiz (University of Twente)

Title: **[Plen03] Chemical Recycling of Packaging Plastic Waste via Thermal Pyrolysis**

Bio: M. Pilar Ruiz is Associate Professor at the Sustainable Process Technology group at the University of Twente, The Netherlands. She holds a PhD in Chemical Engineering and has both industrial and academic experience in the field of chemical technology for sustainable processes. Specifically, her research focuses on developing chemical processes for thermochemical and catalytic conversion of complex feedstocks, such as lignocellulosic biomass and plastic waste. She has (co-)authored over 45 scientific papers and 6 industrial patents. She is also board member of the Dutch Process Technology (NPT) Association.

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Author: Andrea Ramirez (Delft University of Technology)

Title: **[Plen04] Defosilizing the Industrial Sector: From Incrementalism to Radical Disruption**

Bio: Dr. Andrea Ramírez Ramírez is professor of Low Carbon Systems and Technologies in the Faculty of Technology, Policy and Management at Delft University of Technology. She holds a bachelor’s in chemical engineering, a master’s in human ecology, and a PhD in the field of industrial energy efficiency. Her research aims to support the defosilization of industrial clusters by developing and testing methodologies that can be used to identify and assess impacts, synergisms and bottlenecks of deploying novel technologies at industrial and system level. The research combines bottom-up assessment of novel technologies (e.g., reactions, yields, products, operation conditions) with a systematic evaluation of horizontal and vertical interdependencies in dynamic industrial systems. The research is interdisciplinary in character and integrates her chemical engineering background with ex-ante techno-economic analysis, environmental life cycle assessment and system analysis. Prof Ramírez is champion (boogbeld) of the NWA Energy transition route. She has (co-) authored over 115 publications and is Editor-inChief of the International Journal of Greenhouse Gas Control.

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Author: Peter Veenstra (Shell)

Title: **[Plen05] Accelerating Pathways to NET-ZERO: Development of Electro(-Chemical) Driven Reactors/Separators**

Bio: Peter Veenstra is Senior Principal Science Expert at Shell. Peter’s roles include experimentation in the lab, design and commissioning of new (reactor, heat transfer, mixing, separation, transport, energy) technologies, technical services to all businesses, operation in many different countries across the globe, and modelling of technologies and processes. Further career experiences are in fundamental research, research collaborations, international joint industry projects, advisory councils of companies and research projects at national and continent level and venture capital investing support. He served for 8 years as chair of the industrial advisory board of the JM Burgers Centre for fluid mechanics and is member of the selection committee of the national science agenda (Nationale Wetenschaps Agenda) in The Netherlands

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Keynote

Author: Adrie Straathof (TU Delft)

Other Authors: Chema Jimenez Gutierrez, TU Delft; Tamara Jankovic, TU Delft; Tony Kiss, TU Delft; Luuk van der Wielen, TU Delft

Title: **[K01] Efficient pretreatment of lignocellulosic biomass with hot liquid water for co-product valorization**

Abstract: Lignocellulosic biomass provides excellent opportunities for obtaining fermentable carbohydrates, which can be microbially converted into ethanol or any other valuable metabolic product. The solubilisation of the carbohydrates involves physicochemical pretreatment. This leads to co-production of fermentation inhibitors such as acetic acid, furfural, and 5-hydroxymethylfurfural (HMF). In this work, we have studied options to valorize these co-products, and focused on acetic acid recovery. For this reason, we used poplar biomass, which has a relatively high content of acetyl ester groups (about 4 wt%). To pretreat poplar biomass, we selected liquid hot water (LHW) pretreatment, which avoids addition of chemicals that might interfere with subsequent recovery of acetic acid. Batch LHW pretreatment (~ 180 oC, ~ 2 h) hydrolyses most of the hemicellulose in the biomass, and completely hydrolyses the acetyl esters to acetic acid, while lignin and cellulose are not much affected. This pretreatment reaction time is acceptable, especially considering the much longer reaction times for subsequent enzymatic cellulose hydrolysis and carbohydrate fermentation. Upscaling was done by a factor 500 from laboratory to pilot plant. Reaction progress was the same if the heating-up profile was kept the same. A kinetic model was developed to describe the rate of acetyl hydrolysis. Since the reaction is temperature-dependent and catalysed by H+, hence by the released acetic acid, the model included the heating, cooling, thermal expansion, and pH of the reaction mixture. A good fit to the experimental data of acetic acid generation was obtained, but the simulated values of pH were lower than experimentally observed. Buffering by some compounds in the biomass was assumed to occur. Nevertheless, using additional acetic acid as catalyst was shown to be favourable. However, LHW pretreatment cannot avoid hemicellulose degradation products such as furfural, HMF, formic acid, and levulinic acid, in addition to acetic acid. Besides, after solids removal, we reached only low concentrations of solutes (>96 % water). Nonetheless, an effective downstream processing was developed, based on rigorous simulations in Aspen Plus, which allows profitable co-product recovery. About 78.8 % of acetic acid from initial liquid was obtained as a high-purity product (99.8 wt%), while the rest was recycled, together with most of the water, to the biomass pretreatment step. Recoveries of formic acid, furfural and HMF were higher than 99.5 % and product purities satisfied market requirements (73.6 wt% formic acid, 97.9 wt% furfural and 100 % HMF).

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Author: Jan Harmsen (Harmsen Consultancy B.V.)
Other Authors:

Title: **[K02] Teaching break-through process concept design by functions**

Abstract: Break-through process designs have been achieved in industry a few timings by applying functions rather than designing with unit operations. These designs have been implemented at industrial scale and appeared to be lower in cost, energy, and also more reliable. Academic teaching process design using functions however is not a common practice yet. As a consequence, the method is also hardly applied in industry yet. Here a 5-step approach to facilitate process concept design teaching is presented. The steps are: 1 Input and output stream definition. Step 2: Design of streams for recycle, solvent action and extraction. Step 3: reaction and separation function design. Step 4: Heat stream integration design. Step 5: Integrating functions and streams where feasible and selecting unit operations for remaining functions [1]. The steps are not strictly sequential. Often iterations over the steps are made to improve the design. This process concept design method is a synthesis of three process concept design approaches. These are: The Douglas approach with his hierarchy method to first define the input, output and recycle stream structure [2], The Smith approach with his onion model of process concept design, that starts with reactor design, then distillation, then recycle structure design, and finally heat exchange structure [3]. The Siirola approach which is based on functions. Functions are defined to connect input streams to output streams. Iterations are recommended to optimise the concept design. A final step is combining functions and streams as much as possible. He applied his approach successfully for an industrial scale methyl acetate process reducing 11 unit operations a reactive extractive distillation column [4]. It is recommended that academic education trials are carried out with the proposed method. The articles by Rivas may help to define the education courses [5]. In the end the method could be implemented in academic chemical engineering programmes. The method can also be applied in industry. There, very complex process designs can be represented in simple block-flow diagrams by clustering several process steps in a few function blocks with a few input and output streams. For instance a waste water treatment process and a coupled heat pump to provide district heating can be represented in two blocks, facilitating communications between symbiosis partners [6].

References

[1]Harmsen Jan, Verkerk, Maarten. Process Intensification: Breakthrough in Design, Industrial Innovation Practices, and Education. De Gruyter, Berlin, 2020.
[2] Douglas JM, Conceptual design of chemical processes. New York: McGraw-Hill; 1988 Feb.
[3] Smith R, Chemical process: design and integration. John Wiley & Sons; 2005 Jun 10.
[4] Siirola JJ, Industrial applications of chemical process synthesis. In Advances in chemical engineeringing

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Author: Mar Pérez-Fortes (TU Delft)

Other Authors: Josephine Vos, TU Delft; Thijmen Wiltink, TU Delft; Andrea Ramirez, TU Delft; Marula Tsagkari, TU Delft; Sanghamitra Chakravarty, TU Delft; Ibo van de Poel, TU Delft; Hans de Bruijn, TU Delft

Title: **[K03] Multiscale and multidisciplinary modelling for the sustainable design of co-electrolysis systems**

Abstract: The electrolysis or electrochemical reduction of CO2 and water converts these two streams into chemicals using electricity. Depending on the phase of the electrolyte, liquid or solid, electrolysers can be classified as low- and high-temperature electrolysis technologies. Up to date, both technologies are being developed for the co-electrolysis of CO2 and water into a wide range of products. However, the potential of both technologies at an industrial scale remains uncertain; it may be due to heterogeneous methodological assumptions (in experimental/modelling and techno-economic assessments), or assumed optimistic operating conditions (like continuous mode of operation, current or lower-than-current prices, and costs). The environmental and social impact of co-electrolysis are also uncertain and rarely explored. To address this gap, the two Dutch-funded projects, “Addressing the multiscale challenge of CO2 electrochemical reduction” and “Sustainable design of multiscale CO2 electrochemical conversion” (concluding at the end of 2025) aim to contribute to the state-of-the-art knowledge on the optimal scale and conditions for co-electrolysis implementation, by evaluating different (i) process and (ii) supply chain configurations, (iv) business models, and socio-economic strategies, by combining the insights of a multidisciplinary approach. The current work refers to the preliminary results obtained until approximately mid-2023. A “white-box” model for co-electrolysis at high-temperature has been developed in gPROMS, to mainly avoid fundamental errors and misconceptions arising from extrapolating experimental data at the laboratory scale when including such an electrolyser model in a process model. At a process level, an ex-ante techno-economic assessment of the pre-treatment units for purifying CO2 from different sources has been performed, as an initial step towards the modelling in Aspen Plus of a complete solid-oxide electrolysis-based plant that produces syngas. The required CO2 purity levels for high-temperature electrolysis have been compared to the required CO2 purity levels for low-temperature electrolysis. At a supply chain scale, a facility location model has been built in GAMS to gain an understanding regarding centralised/decentralised configurations for co-electrolysis plants; i.e the influence of the capacity of the plants that produce syngas and of CO2 and syngas transport costs, on the central/decentral placement of these plants. At a system level, interviews with relevant stakeholders along the whole value chain have taken place. This information has been used to identify the relevant sustainability-related values that are crucial to consider at early design stages and to identify relevant stakeholders and related barriers and enablers for the implementation of co-electrolysis plants.

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Author: Kees Maarschalk (Avebe)

Other Authors:

Title: **[K04] Technology: a crucial component in food transition. How a Dutch co-operative contributes to more sustainable foods**

Abstract:

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Author: Armin Fricke (CGC Capital-Gain Consultants GmbH)

Other Authors: Jwal Soni, CGC Capital-Gain Consultants GmbH; Luisa Malek, CGC Capital-Gain Consultants GmbH; Daniel Wagner Oliveira de Medeiros Self-employed, Manaus/ Brazil

Title: **[K05] Python in Chemical Process Simulation**

Abstract: Python is a powerful programming language that has become increasingly important in the field of chemical engineering. One reason for its growing popularity is its versatility and ability to handle a wide range of tasks. It offers libraries, such as SciPy and NumPy to perform complex mathematical calculations, or libraries for data analysis, such as pandas and scikit-learn to work with large sets of data. Despite its many strengths, Python is not currently able to fully replace specialized process simulation software in chemical engineering. These simulation software packages, such as Aspen Plus, HYSYS, CHEMCAD, ProII and DWSIM, have been developed specifically for use in the chemical industry and have many more advanced features than those available in Python libraries. For example, they may have more detailed thermodynamic models, a more comprehensive library of chemical compounds, or pre-built unit operations, e.g., distillation columns and reactors. There are several ways to integrate Python with a chemical process simulator depending on the specific chemical process simulator being used and the desired level of integration. Directly integrating Python with a chemical process simulator by using its Application Programming Interface (API) allows to run the chemical process simulator and automate it with Python scripts.
This enables to combine simulator-internal and external optimizers creating complex simulations that can be used to analyze and predict chemical processes, which aids in the design and optimization of chemical processes, leading to more efficient and sustainable, and cost-effective production. This contribution shows how HYSYS, CHEMCAD, and DWSIM can be used from Python to create surrogate models (SM) from flowsheet simulations (PFD), embed SM in PFDs, optimize PFDs using SM, and create new PFDs using AI assistance.

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Author: Michael Wartmann (Nouryon Chemicals B.V.)

Other Authors:

Title: **[K06] Designing Chemical Manufacturing Automation with Care**

Abstract: Manufacturing processes have increasingly become automated over the past decades. Starting out with small-scale hand-operated processes in the early times, current state of the art can in specific cases reach near autonomy and remote operation for large and complex processes. The drive for automation is twofold: Primarily, improving the productivity of the process by lowering cost and increasing throughput ever further involving advanced sensors, computer models, and algorithms. On the other hand, finding ways to enhance plant and operator safety, ergonomics, and general reliable operability of the respective process plant. This drive for automation has led for the common process operators, engineers, and managers to transition from their work being a craft with significant freedom of design to an increasingly passive and procedural professional frame with few but potentially severe exceptions during abnormal operation. In this work, I discuss how technology relations in technology-mediated organizations often unknowingly and implicitly choose for an ethical perspective by the way automation technology is adopted. Realizing the causality dilemma of a human organization and its applied technology being tightly intertwined, I propose reevaluating the perspective on automation in industry. Automation requires balancing the concept of Heidegger's releasement in combination with critical thinking towards an ethical dialogue throughout all technology design phases. In this design approach, technological maturation runs in parallel to psychological maturation of the workforce and their leadership. Eventually, organizations can adopt concepts such as Nussbaum and Sen's capability approach helping them define their ethical perspective of care for workforce, customer, society, and nature leading to sustainable technology deployments. These technology-mature organizations would understand the fundamental nature of human-technology relations and design for it through having creative capabilities of the connected individual expressed, understood, and mediated and realizing that technology is an extension of humanity and out ethics rather than a neutral tool.

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Author: Albert Santoso (TU Delft)

Other Authors: Svenja Trapp, TU Delft; Robin de Kruijff, TU Delft; Elisabeth Paulßen, Aachen University of Applied Science; Volkert van Steijn, TU Delft; Ruud van Ommen, TU Delft

Title: **[L01] Liquid-liquid extraction of medical radioisotopes in microfluidic channels treated by atomic layer deposition**

Abstract: In the field of cancer diagnostics, there is an increasing interest in using shorter half-life medical isotopes such as 68Ga and 86Y. Within ten of hours, most of these isotopes decay to a less usable form, leading to minimization of unwanted doses towards the patient. Furthermore, these isotopes are also easy to be labelled, making it interesting radiopharmaceuticals for on-demand use in hospitals. However, this exact short half-life property poses challenges in the production route. After the initial target materials are being irradiated by the cyclotron, these radioisotopes have to be quickly and efficiently isolated. Currently, ion exchange chromatography is used and it takes up to several hours to be performed. As a result, the final eluted product tends to have low overall activity, making this isotope less viable. To address these problems, we propose microfluidic liquid-liquid extraction which is known for both improved mass transfer and possible fluid profile manipulation compared to batch processes. In this study, two elements were studied: Ga and Y. We used polydimethylsiloxane (PDMS) parallel-flow microfluidic chips to selectively extract Ga and Y elements from the target solution consisting of Zn(NO3)2 and Sr(NO3)2 (in 10mM HNO3)respectively. As the extracting phase, we use chelating agent (BPHA and/or D2EHPA) in an organic solvent (chloroform and/or 1,8-cyneol). To protect the PDMS from chemical swelling, we deposited a nanolayer of SiOx internally in the chip (i.e., on the channel wall) using atomic layer deposition (Santoso et.al., ChemComm, 2022). The result shows that by using vertical and lateral pinning hooks, defined parallel flows with 99.9% fluid disengagement was achieved within a relatively challenging flowrate range (Capillary number of 10-5 to 10-3). The preliminary experiment resulted in 98%±2% extraction efficiency of natGa after contact time of 30 seconds and 99%±1% extraction efficiency of natural Y after contact time of 10 seconds. When we followed up with active 68Ga at lower concentrations but with similar contact time, 85% efficiency was achieved. This study shows not only a promising method of extracting short half-life isotopes efficiently, but also a possibility to directly recycle expensive, enriched target solutions. This publication is part of the Open Technology programme financed by the Dutch Research Council (NWO).

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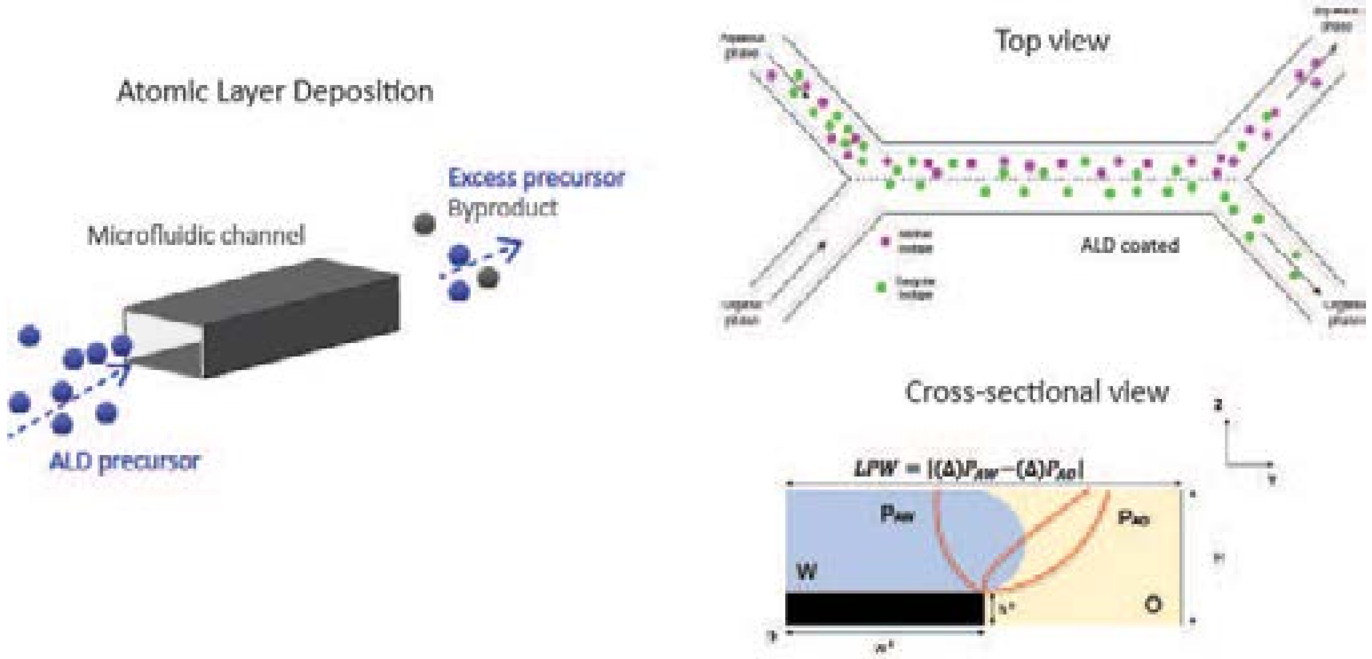

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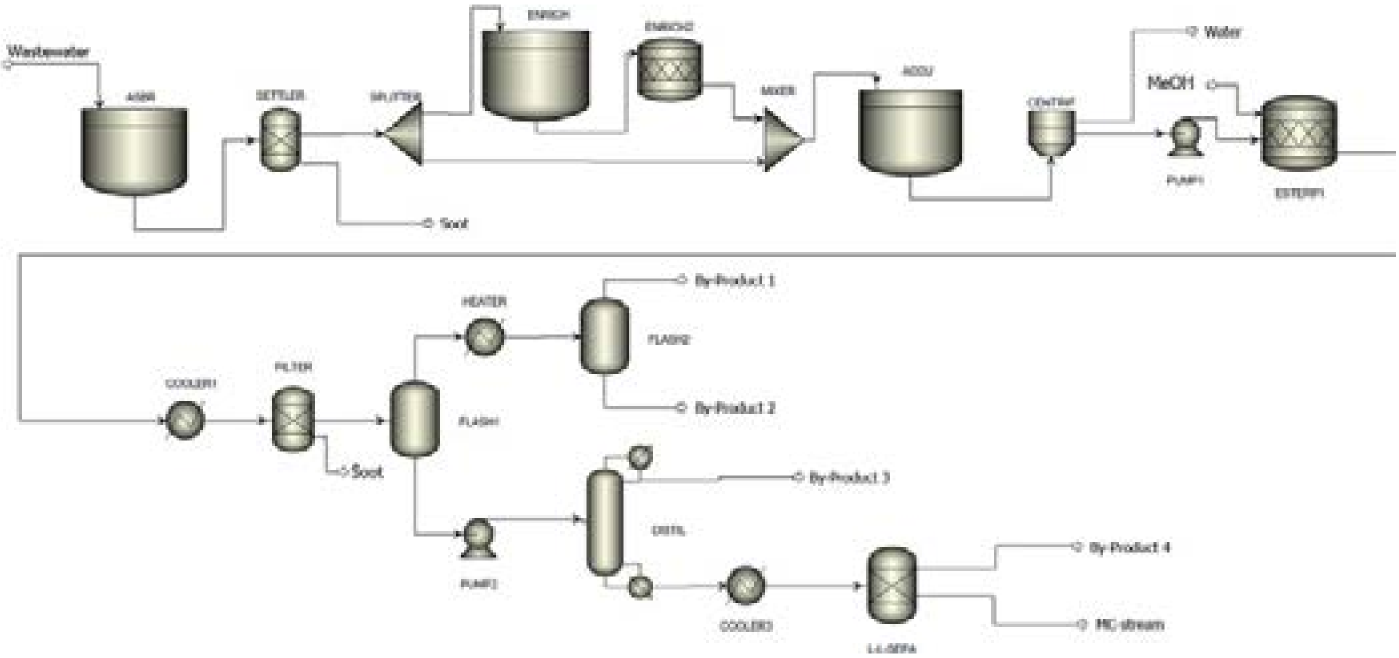
Author: Akbar Asadi Tashvigh (WUR)

Other Authors: Joris Koch, Elinor Scott, Johannes Bitter, Akbar Asadi Tashvigh

Title: **[L02] A plant wide simulation of polyhydroxyalkanoate production from wastewater and its conversion to methyl crotonate**

Abstract: This work simulates the production of methyl crotonate from various industrial wastewaters. In the upstream process, wastewater is fermented into volatile fatty acids which are then converted into polyhydroxyalkanoates (PHA) by means of mixed microbial cultures. In the downstream, PHA undergoes a series of thermolysis and esterification reactions to produce methyl crotonate. The origin of the wastewater was found to have a great influence on the composition of the PHA with the effluent of a candy bar factory producing a high polyhydroxybutyrate/polyhydroxyvalerate ratio of 86/14 in favour of methyl crotonate production. It was observed that the use of intracellular polyhydroxybutyrate, instead of purified, significantly lowers the number of separation steps and yet reduces the methyl crotonate recovery by only 20 %. An operating pressure higher than 18 bar led to more transesterification of polyhydroxybutyrate, producing byproducts instead of methyl crotonate. Finally, a 3 h reaction was found sufficient for completion of polyhydroxybutyrate conversion.



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Author: Lars Puiman (TU Delft)

Other Authors: Eduardo Almeida Benalcazar, TU Delft; Henk Noorman, Royal DSM, TU Delft; Cees Haringa, TU Delft

Title: **[L03] Coupling hydrodynamics and metabolic dynamics in syngas fermentation guiding industrial reactor design**

Abstract: Syngas fermentation is a promising commercial process for converting gaseous waste streams with significant CO and H2 content into added-value chemicals. Currently, it is commercialized by a handful of companies; amongst them, LanzaTech employs an external-loop gas lift reactor (EL-GLR) for converting off-gases into ethanol. The typical gas and liquid flow pattern in such reactors was found to lead to frequent oscillations in dissolved gas concentrations, from the microbial point of view. A two-way coupled Euler-Lagrangian CFD model was deployed to study how the oscillations in the dissolved gas concentration (Figure 1a) would affect individual cells and the global reactor performance. A recently developed lumped (linlog-based) metabolic kinetic model was coupled with a multiphase CFD model, to obtain results with a high spatio-temporal resolution from both the reactor and the microbial perspective. The dynamic kinetic model describes 12 compounds and 11 intracellular reactions, while the CFD model describes the fluid flow, turbulence and mass transfer in the industrial-scale EL-GLR.

This model was used to describe how large-scale dynamics would affect the biomass-specific ethanol productivity, cellular CO and H2 uptake rate, and the intracellular metabolite concentrations. The model predicts that there is a typical delay in the seconds range between gas uptake and ethanol production. This time period is mainly used for the conservation of energy, i.e., orderly: harvesting electrons from the gas substrates, generation of the proton motive force and secretion of products. In the large-scale reactor simulation, these mechanisms led to specific zones with high metabolic activity wherein high intracellular concentrations of reduced ferredoxin were predicted (Figure 1b), which is used as an intracellular storage pool for electrons originating from the substrate gases. When the cells are rich in ferredoxin, the excess electrons are being used for the production of ethanol. This happens at the top section of the reactor, where the reduced ferredoxin is oxidized and where high biomass-specific ethanol production rates were observed (Figure 1b,c). We also revealed zones with low metabolic activity, such as the end of the downcomer, due to depletion of intra- and extracellular electron sources. This two-way coupled CFD-CRD model for syngas fermentation offers new fundamental insights into the microbial behaviour in large-scale syngas fermentation that can inspire further experimental investigation, and opens the way towards rational optimization of operating conditions and reactor design, for increased ethanol productivity in industrial syngas fermentation processes.

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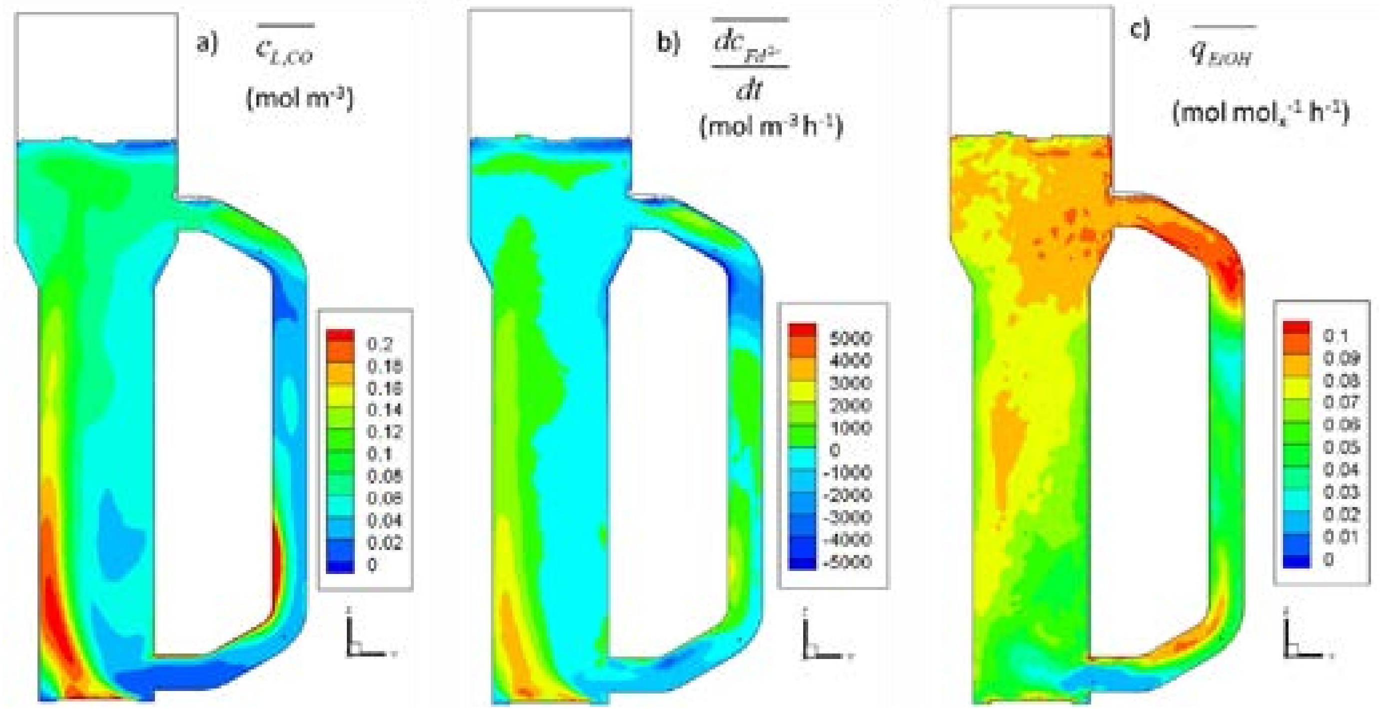

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Author: Tamara Janković (TU Delft)

Other Authors: Adrie J. J. Straathof, TU Delft; Anton A. Kiss, TU Delft, TU Delft

Title:

[L04] Eco-friendly recovery of valuable by-products for enhancing hot-liquid water pretreatment of biomass

Abstract: Lignocellulosic biorefineries potentially present great renewable alternative for biofuel production. One way to increase their competitiveness is to enhance the pretreatment step, which is needed due to the complex structure of lignocellulosic biomass. With relatively low costs and mild process conditions, hot-liquid water pretreatment is an environmentally friendly method. However, the value of the liquid remaining after this step is usually neglected. Therefore, this research focuses on adding value to this otherwise waste stream. The main goal is to recover generated by-products from this liquid, such as acetic acid, formic acid, furfural and 5-hydroxymethyl furfural (HMF). Recovery of mentioned components via different methods has been proposed. Notwithstanding, recovery yields are often insufficiently high, addition of extra chemicals complicates downstream processing and research is usually done only on lab-scale, without scaling-up. Therefore, distillation is chosen as the main separation technique for by-products recovery process. Aspen Plus is used to effectively develop simulations for every process operation. The major difficulty in this research is highly diluted solution (>96wt% water) remaining after the pretreatment step, as well as thermodynamic constrains due to the formation of three azeotropes (water – furfural, water – acetic acid – formic acid and water – formic acid) and tangent pinch in aqueous acetic acid mixtures. The unique contribution of this work is an optimal process design for recovery of acetic acid, formic acid, furfural and HMF. All recovered product are obtained in forms that satisfy market requirements, whereby the purities of product streams are 99.8wt% acetic acid, 73.6wt% formic acid, 97.9wt% furfural and 100wt% HMF. About 78.8% of initially present acetic acid is recovered as high-purity product, while the rest of it, together with most of the water, can be recycled to the biomass pretreatment step in order to increase biomass digestibility. Recoveries of formic acid, furfural and HMF are higher than 99.5%. Mechanical vapor recompression and heat integration are implemented in order to decrease total energy use. This results in the following benefits: 88.0% reduction in primary energy requirements (from 75.13 to 8.99 kWh/kgproduct), 82.7% reduction in CO2 emission (from 10.84 to 1.88 kgCO2/kgproduct) if used electricity is from non-renewable sources, or as much as 99.7% reduction (to only 0.03 kgCO2/kgproduct) if green electricity is used and 95.7% reduction in cooling water consumption (from 12.93 to 0.55 m3/kgproduct). Additionally, despite 93.7% increase in total capital cost (from 24923 to 48284 k$), 85.5% decrease in total operating costs (from 2.29 to 0.33 $/kgproduct) leads to about 76.6% decrease in total annual costs (from 2.41 to 0.56 $/kgproduct). Summing up, the novelty of this research is an optimal eco-friendly recovery process of valuable by-products after the biomass pretreatment step..

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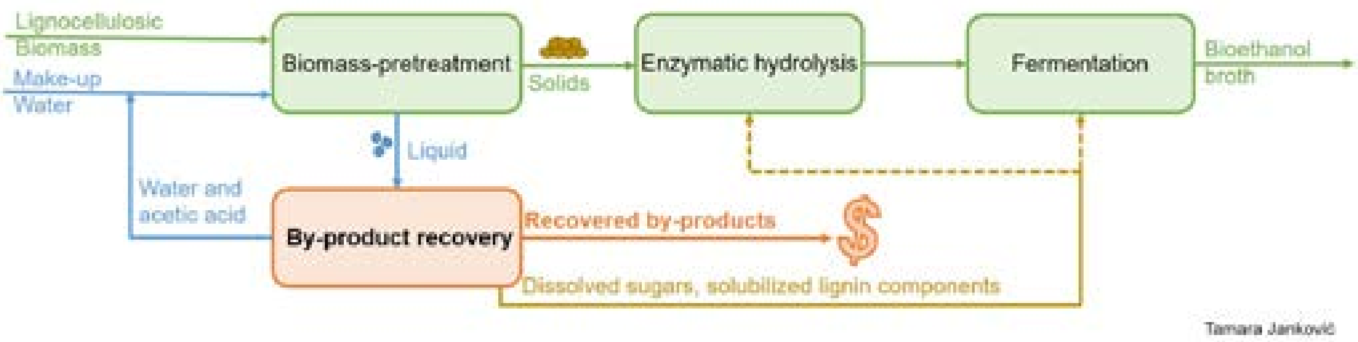

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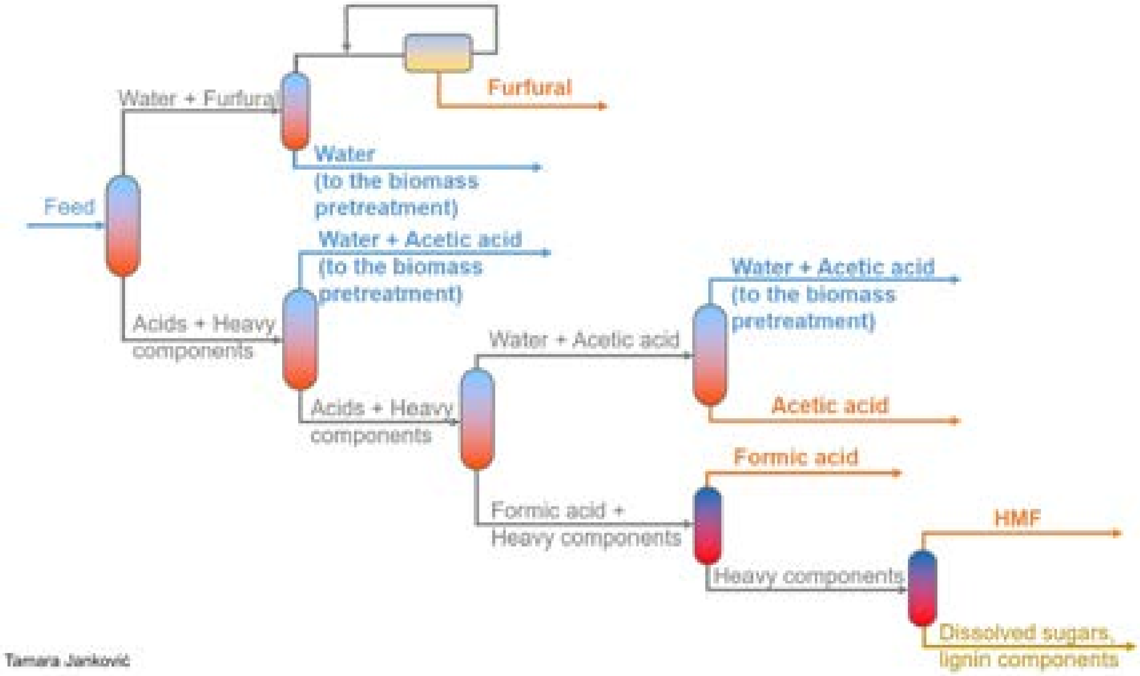

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Author: Jord Peter Haven (UTwente)

Other Authors: Jimmy A. Faria Albanese, University of Twente; Leon Lefferts, University of Twente

Title: **[L05] Industrial Production Of Propylene Using Dense Ceramic Membranes**

Abstract: Propylene is a widely used chemical building block that is conventionally produced via cracking processes. A more direct route to produce propylene is via non-oxidative dehydrogenation of propane ($C3H8 \leftrightarrow C3H6 + H2$, $\Delta H = +124.3$ kJ/mol), which can be achieved using Pt-supported catalysts [1]. However, propane dehydrogenation (PDH) requires high temperatures (500-700 °C) and is limited by thermodynamic equilibrium (propylene yield: ~30%), which makes existing industrial PDH processes highly energy-intensive [1]. The energy intensity of industrial PDH processes and thereby the corresponding CO2 emissions can be strongly reduced by shifting the equilibrium towards the propylene side. This can potentially be achieved by using H2 permeable dense ceramic membranes [2]. Two types of dense ceramic membranes exist: (i) mixed proton-electronic conducting (MPEC) membranes, and (ii) purely proton conducting membranes. In the former, hydrogen transport is driven by a gradient in H2 chemical potential, whilst in the latter hydrogen transport is driven by a combination of a gradient in H2 chemical potential and a gradient in electrostatic potential due to the application of an external voltage. MPEC membranes allow for slightly higher propylene yields, but a sweep gas is needed to minimize permeate side H2 chemical potential to drive H2 permeation, yielding a low pressure diluted H2 byproduct. Purely proton conducting membranes allow for considerably higher propylene yields, due to the electrical driving force, and have the advantage of yielding a pure H2 byproduct stream at elevated pressure. In this contribution, three different industrial PDH processes are compared to each other in terms of CAPEX, OPEX, energy usage, and CO2 emissions: (i) a conventional PDH process, (ii) a PDH process driven by MPEC membranes, and (iii) a PDH process driven by purely proton conducting membranes. These three processes are simulated in Aspen Plus and the CAPEX, OPEX, and energy usage requirements are determined per unit operation after heat integration. Initial insights show that electrically-driven membrane processes can be considerably more sustainable (in terms of CO2 emitted per ton of propylene) than the conventional process, but will be more costly because of the high costs of the membrane reactor itself.

References

1 Sattler, J.J.H.B., Ruiz-Martinez, J., Santillan-Jimenez, E., Weckhuysen, B.M., Chem. Rev. 114, 20 (2014)

2 Deibert, W., Ivanova, M.E., Baumann, S., Guillon, O., et al. J. Membr. Sci. 543 (2017)”

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Author: Eduardo Francisco Almeida Benalcázar (TU Delft)

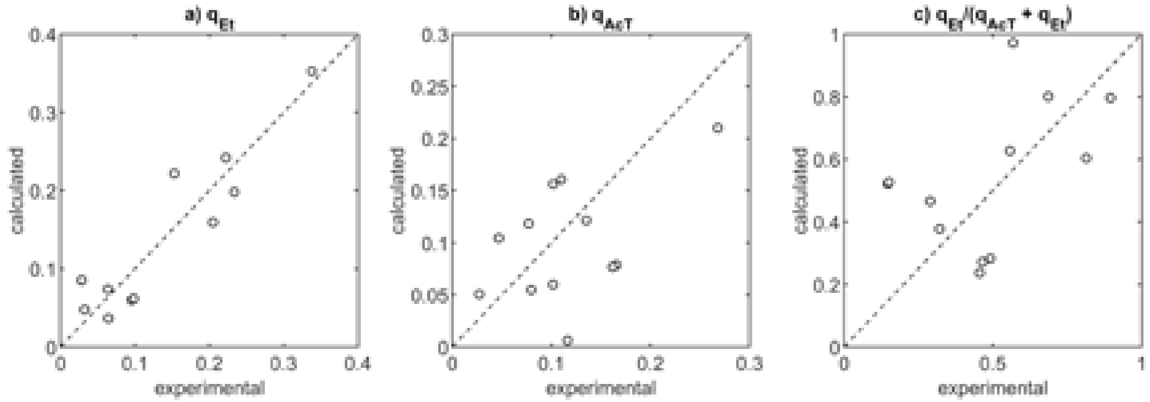
Other Authors: Sef Heijnen, TU Delft; Rubens Maciel Filho, State University of Campinas; John Posada, TU Delft; Henk Noorman, TU Delft / Royal DSM

Title: **[L06] Modeling of syngas fermentation: a Gibbs free energy-constrained black-box model that predicts selectivity between ethanol and acetic acid**

Abstract:

This work presents the development of a black-box model of the bacterium Clostridium autoethanogenum. The model is assembled for the simulation of ethanol, acetic acid and 2,3-butanediol production from the anaerobic fermentation of CO, H2 and CO2. The necessary input data are the concentrations of substrates and products in the extracellular space and model's outputs are the specific net conversion rates, or q-rates. The model is aimed at reproducing common conditions by which ethanol production is favored over that of acetic acid, i.e., low pH, high acetic acid concentration and use of H2-rich gas mixtures.

The model is calibrated using reconstructed steady state data gathered from 12 published continuous fermentations with C. autoethanogenum employing several ratios of CO and H2 in the gas feed, several gas mass transfer rates and two dilution rates. The modeling approach here presented contains two special features, i) it considers cells growth under dual-limiting substrate conditions, where CO and the H2/CO2 pair are both limiting substrates, and ii) it uses the rates of Gibbs free energy production by metabolism to derive information about the energy aspects of different intracellular processes, including growth, acetate export and acetic acid diffusion into the cells. The model is used to i) extract design information from previously reported fermentations at pseudo steady state, ii) identify possible reasons behind the preference of CO and H2 consumption when both electron donors are present in the gas feed, iii) assess the consequences of choosing different mechanisms for the active export of acetate, and iv) evaluate the presence of a H2 production and consumption futile cycle. The integrated model is able to accurately reproduce common experimental observations where ethanol production is favored when pH is low, acetic acid concentration is high, and rate of H2 uptake is faster than CO uptake.



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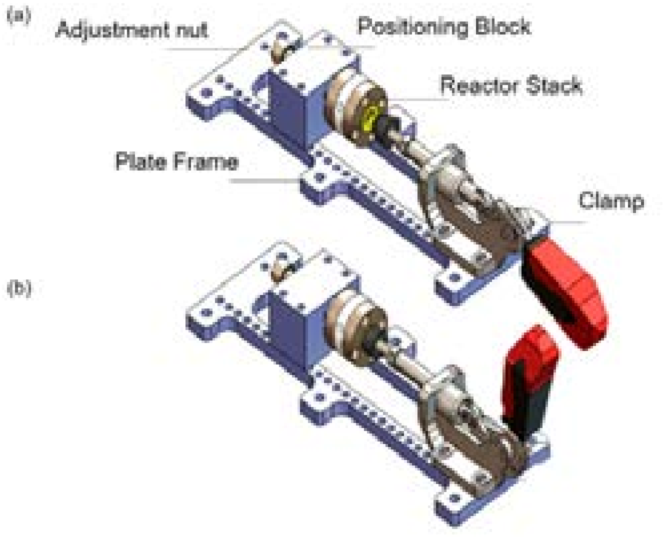
Author: Nandalal Girichandran (TU Delft)

Other Authors: Dr. Andrew Morrison, University College London; Quincy Wols; Dr.Ruud Kortlever TU Delft

Title: **[L07] Design of an Elevated Pressure Electrochemical Flow Cell for CO2 Reduction**

Abstract: Electrochemical CO2 Reduction (ECO2R) has already been established as a sustainable way of closing the carbon cycle while synthesizing useful commodity chemicals. One of the favourable routes to scale up the process is the elevated pressure ECO2R because it is one way to increase the concentration of the poorly soluble CO2 in aqueous systems. Yet, there are not many studies that focus on it owing to the inherent challenges with high pressure systems such as leaks, product quantification, ease of operation etc. In this study, a novel high pressure flow cell setup has been designed and validated. The modular design uses a clamp system, which facilitates easy stacking of multiple cell parts while being capable of handling pressures up to 50 bar. The effects of CO2 pressure on the reaction were investigated on a gold (Au) foil cathode in 0.1M KHCO3 electrolyte. We successfully measured gaseous products using an inline Gas Chromatograph where the selectivity towards CO enhanced, as the pressure was increased from 2 to 30 bar. The reported setup provides a robust means to conduct high pressure electrolysis experiments in an easy and safe manner, making this technology more accessible to CO2 research community. In the future, this flexible design could facilitate the study of ECO2R under pressure, paired with other electrolyzer types like the zero-gap, GDE, or bicarbonate electrolyzers, at industrially relevant current densities.



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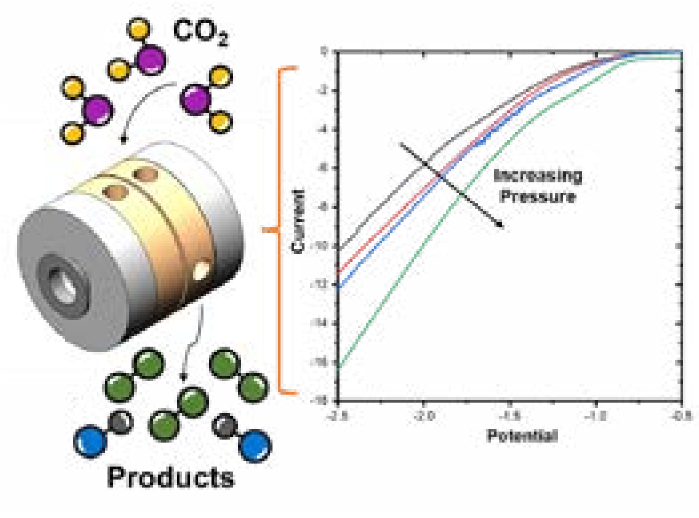

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Author: Anirudh Venugopal (HyET E-Trol)

Other Authors:

Title: **[L08] Development of high differential pressure AEM electrolyzer**

Abstract: Green hydrogen is considered as an important vector for decarbonisation in this on-going energy transition. Green hydrogen will find applications in the hard to abate sectors like chemical industries, heavy duty transportation, large scale power storage and transport, green steel and fertilizer production etcetera. To make this transition economical and self-sustainable, the cost of green hydrogen has to be lower or at least on par with the cost of hydrogen produced from fossil-based sources. Drastic innovations in the way we produce and process green hydrogen are required to drop the cost of green hydrogen multi-fold and make it cost competitive. Improvements in the system efficiencies and a decrease in capital costs are both required to enable this. The cost of post-processing of hydrogen gas, which includes compression, accounts for about 30% of the sale cost of green hydrogen. Mechanical compressors used in such systems are a mature technology and hence, drastic performance improvement and cost reduction with the scale-up of such a technology is not expected. In addition, mechanical compressors require very high maintenance, have a high down time and are not suited for dynamic and intermittent operations. These factors will also influence the cost of green hydrogen. Therefore, new innovative technologies are required to produce high pressure hydrogen that will significantly decrease the cost of green hydrogen production, while requiring low maintenance and being suitable for dynamic and intermittent operation. HyET E-Trol is developing a novel high differential pressure AEM electrolyzer that can directly output hydrogen at pressures upto 200 barG. Such integrated electrolyzer systems are expected to decrease the capital costs of the system by atleast 35% and improve the overall system efficiency by more than 40%, in comparison to the current state of the art systems. The anion exchange membrane technology also makes uses of more sustainable and abundant materials for the stack construction in comparison to the current SoA technologies. In this talk, current progress in the development of this technology and the impact this technology can have in the future hydrogen market will be discussed.

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Author: Nathalie E.G. Ligthart (TU Delft)

Other Authors: Gerard Prats Vergel, TU Delft; Mohammed A. Khan, TU Delft; David A. Vermaas, TU Delft; Johan T. Padding, TU Delft

Title: **[L09] Suspension electrodes for electrochemical CO2 reduction**

Abstract: CO2 capture and conversion is an important part of the energy transition towards green electricity and clean fuels. However, low solubility of CO2 in water and it's slow diffusion cause mass transfer limitations in electrochemical CO2 reduction. This significantly lowers the current densities at which high Faradaic efficiency towards the desired product can be reached during the reaction in water. Enhancing mass transfer and raising the limiting current density is a challenge and an important step towards the industrialization of aqueous electrochemical CO2 reduction. We investigate whether mass transport can be improved by using flowable suspension electrodes instead of stationary electrodes. In this work, we perform CO2 reduction on flowable suspension electrodes and study what the requirements are for a well-performing flowable cathode. In order to achieve this, we measure and vary key properties of the suspension and asses their impact on the electrode performance in terms of Faradaic efficiency and limiting current density. Gaining understanding in the design parameters and requirements for flowable electrodes opens up a route to enhance mass transfer in more electrochemical energy conversion processes.

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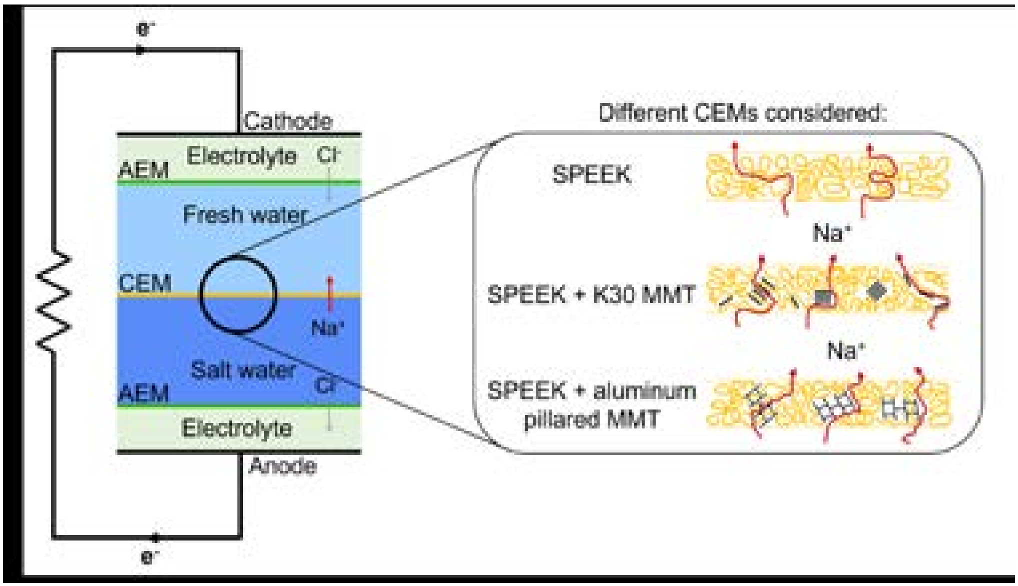
Title: **[L10] Clay composite membranes for salinity gradient batteries**

Abstract: Sodium chloride gradient batteries are attractive urban energy storage solutions thanks to their ability to easily be scaled up and their use of abundant, safe, and cheap materials. However, large scale deployment of this technology is currently hampered by the lack of low-cost ion exchange membranes that have both excellent permselectivity and high ionic conductivity. This problem can be tackled by using composite membranes that combine a cheaper hydrocarbon matrix than the state-of-the-art perfluorosulfonated polymers with the attractive properties of inorganic fillers. In this work, microcomposite membranes made of sulfonated poly(ether ether ketone) (SPEEK) and 1 to 20 wt.% K30 montmorillonite (MMT) and aluminum pillared MMT (Al-pil MMT) are considered. The obtained membranes were heterogeneous microcomposite membranes due to the immiscibility of the naturally occurring clays in the SPEEK matrix. The addition of inorganic clays with 2D geometries enables the introduction of percolating sodium diffusing pathways with reduced tortuosity. As a result, the conductivity of the membranes increases with an increasing clay loading fraction, reaching up to 1.4 times that of the pure SPEEK with 20 wt% K30 MMT. The permselectivity of the SPEEK membrane also improves with the addition of set amounts of K30 MMT, while the Al-pil MMT composites suffer from a slightly reduced permselectivity (by no more than 3%) due to their higher water uptake. This is due to the larger hydrophilic interlayer spacing in the Al-pil MMT which creates more free volumes in the membrane. These results show that the addition of naturally occurring clays to a polymer-based cation exchange membranes is a promising method to improve the permselectivity-conductivity trade-off.



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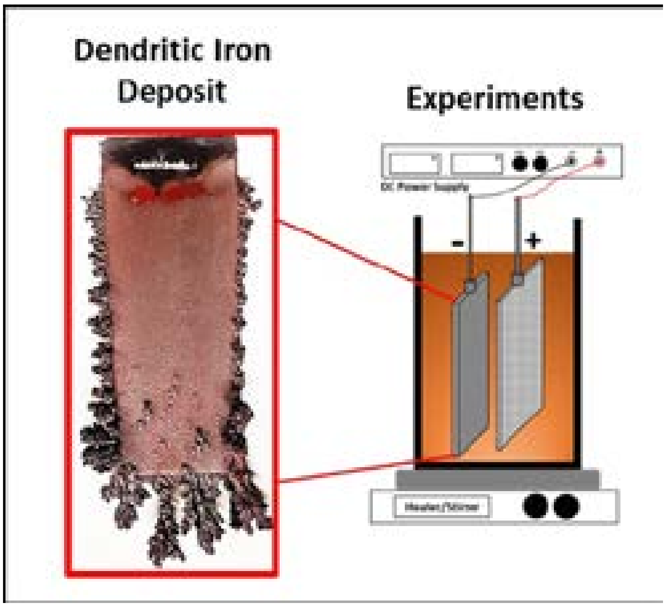
Other Authors: Yali Tang TU/e & EIRES; Giulia Finotello TU/e & EIRES; John van der Schaaf TU/e & EIRES; Niels Deen TU/e & EIRES

Title: **[L11] Dendritic Iron Formation in Low-Temperature Iron Oxide Electroreduction Process using Alkaline Solution**

Abstract: Low-temperature electrochemical reduction (electroreduction) is considered to be a suitable method for iron oxide reduction due to its attractive aspects, such as its CO2-free operation and low electric energy consumption and temperature requirements. Aiming at metallic iron of powder form as product, our research promotes dendritic electrodeposition rather than to grow compact deposition layers as in conventional electrowinning methods. Proof-of-concept experiments are performed using a single parallel plate electrode, immersed in a mixture of micro-sized hematite (Fe2O3) powder and strong aqueous alkaline (NaOH, 50%wt, 18 M) electrolyte. The effects of current density, hematite mass fraction, temperature, and particle size on deposit morphology and Faradaic efficiency are also investigated. It is found out that the dendritic structures are more likely to grow in a non-homogeneous environment, e.g. when experiments carried out without stirring or with local heating. Furthermore, the dendrites are located primarily on the side and edge of the cathode, indicating a diffusion-controlled mechanism. A cathodic deposition of metallic iron with a high Faradaic efficiency (> 90%) is successfully accomplished. The present findings provide new insight into the production of electrolytic iron powder (e.g. in the metal fuel application) and the acceleration of sustainable ironmaking technologies.



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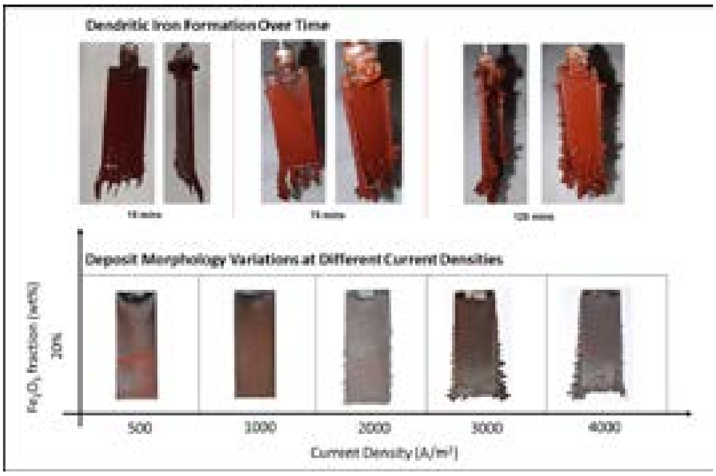

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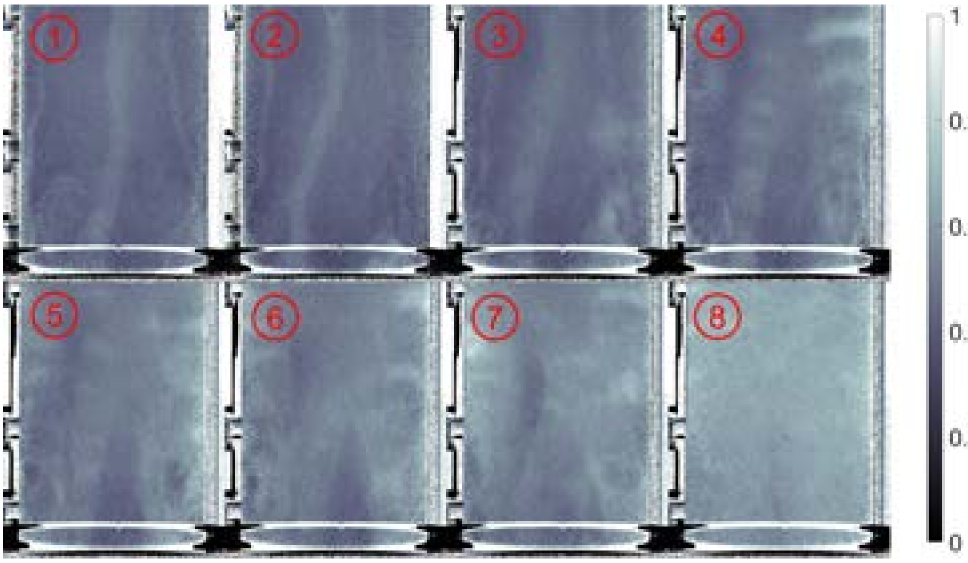
Title: **[L12] The mechanism behind vibro-assisted fluidization of cohesive micro-silica**

Abstract: In sectors such as food, pharma and catalyst manufacturing we see an increasing interest of applying fluidization to particles in the Geldart C range. When it comes to these particles, fluidization becomes challenging due to strong attractive inter-particle forces. This results in channel formation and agglomeration, both of which lead to a reduction in gas-solid contact. To fluidize cohesive particles, assistance methods can be employed, which introduce additional manipulation. For most assistance methods, studies have concluded that the mechanism by which fluidization was improved, is by breaking up agglomerates. We hypothesized that it is not the agglomerates, but the channeling that is targeted by these assistance methods. In this study, we used X-ray imaging to study channel formation and collapse within a fluidized bed of cohesive microparticles. Pressure drop, bed height and off-line agglomerate size measurements were performed as well, to decouple the effect of channel disruption and breaking of agglomerates.

It was observed that channeling is the main cause of poor fluidization of the micro-silica, resulting in poor gas-solid contact and little internal mixing. Improvement in fluidization upon starting the mechanical vibration was achieved by disrupting the channels. Agglomerate sizes were found to not significantly change during experiments.



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Title: **[L13] Stirrer design for improving fluidization of cohesive powders**

Abstract: Fluidization is widely used for a variety of solid processing applications, in which interphase mixing and heat and mass transfer are paramount. Steady fluidization is easily achieved using sand-like powders, whereas it is rather challenging to aerate fine particles because of intrinsic cohesion. Substantial attractive forces between individual grains dominate the collective behaviour, leading to the formation of agglomerates and gas channels which undermine greatly gas-solids interaction. Imposing additional forces and energies to the system is, therefore, necessary to aid fluidization. Several approaches have been studied to boost the fluidization of fine powders [1]. In particular, continuous stirring is shown able to effectively suppress channel formation, as well as mitigate agglomeration [2]. In addition, stirring is in favour of scale-up practices in terms of capital cost, operation and effective area size. Nevertheless, stirrers of different geometries exhibit dissimilar impacts, and there are only limited attempts of the stirred fluidization of cohesive powder. The effects of different stirrer designs remain largely unknown. In this work, we investigate the impacts of stirring on the fluidization of cohesive powders under varying stirrer designs and operating conditions. The fluidization performance was evaluated based on a comprehensive comparison across stirrer blade length, number, torsion angle, thickness and geometry, as shown in Fig.1. X-ray imaging technique was used to monitor the system hydrodynamics, such as gas bubbling and channelling behaviour. We observed that stirring effectively enhances the fluidization of cohesive powder, and mitigates gas channel formation. The experiments show that volume-based stirrers outperform plane-based designs in assisting fluidization. The analysis conducted forms a useful reference to optimise the stirrer design for existing and future applications.

[1] J.R. van Ommen, J.M. Valverde, R. Pfeffer, Fluidization of nanopowders: a review, J. Nanopart. Res. 14 (2012) 737.
[2] S. Alavi, B. Caussat, Experimental study on fluidization of micronic powders. Powder technol., 157(1-3) (2005) 114-120.

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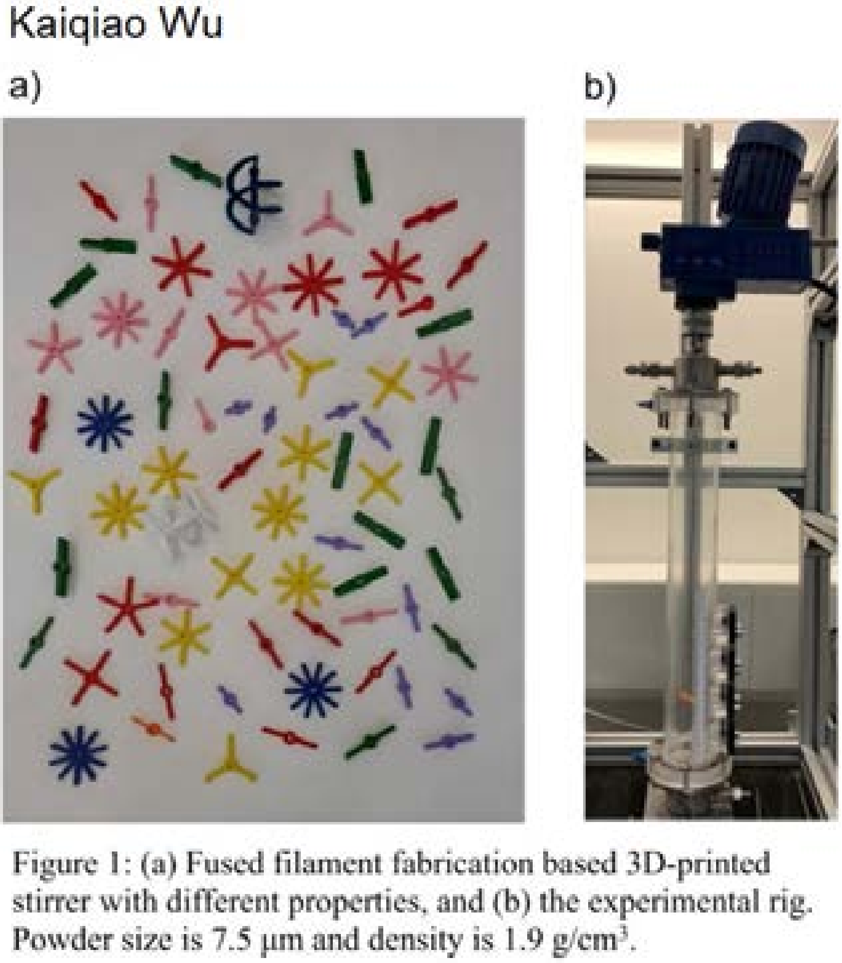

Kaiqiao Wu

Figure 1: (a) Fused filament fabrication based 3D-printed stirrer with different properties, and (b) the experimental rig. Powder size is 7.5 μm and density is 1.9 g/cm^3.

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Author: Pieter Christian van der Sande (TU Delft)

Other Authors: Evert C. Wagner,TU Delft; Gabrie M.H. Meesters, TU Delft; J. Ruud van Ommen, TU Delft

Title: **[L14] Understanding particle flows in sub-fluidized horizontal stirred bed reactors by radioactive particle tracking**

Abstract: Horizontal stirred bed reactors are commercially employed in polypropylene manufacturing processes. The reactors generally contain a bed that is mildly stirred by a series of paddles attached to a center shaft. Via nozzles located at the bottom of the reactor gaseous propylene enters the reactor at controlled flowrate to prevent bed fluidization, bringing the bed in sub-fluidized state. It is crucial to have a well-mixed system with a narrow particle cycle time distribution throughout the reactor to avoid the formation of hotspots that could lead to expensive reactor shutdowns due to lump formation. It is therefore of great importance to understand the particle flows in horizontal stirred bed reactors. In this research, we developed a lab-scale horizontal stirred bed reactor that enables particle flow studies in non-reactive environments. Since optical techniques are inadequate to study the dense flows, we study the reactor hydrodynamics with X-ray imaging and radioactive particle tracking (RPT). Gas-solid distribution maps acquired with X-ray imaging showed that at higher inlet velocities bed spouting occurs, leading to substantial gas by-pass and poor gas-solid interaction. Now we use RPT to characterize particle trajectories in the reactor. The RPT setup consists of three scintillation detectors that form a field of view around the reactor. Within this field of view the location of the tracer particle is reconstructed with sub-millimetre and sub-second accuracy. We studied the effect of the reactor filling, gas inlet flowrate and agitator rotation speed on the particle cycle time distribution and axial dispersion for industrial-grade polypropylene (Geldart B type). We found that at higher reactor fillings and higher rotation speeds the particle has a shorter cycle time, which would lead to improved heat removal in the process. The results from this study contribute to better understanding of the flow behaviour in horizontal stirred bed reactors.

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Author: Lu Zhang (RUG)

Other Authors: Jun Yue, University of Groningen

Title: **[L15] Hydrodynamic study of single- and two-phase flows in packed bed microreactors**

Abstract: Heterogeneously catalyzed reaction accounts for 80-90% of industrial catalytic chemical processes, making packed bed reactors commonly used in the industry. Packed bed microreactors combine the advantages of packed bed and microreactor technology, which can achieve significant process intensification, precise reaction operation, and safety control of catalytic chemical synthesis. In light of this, packed bed microreactors offer a number of opportunities for the effective and sustainable chemical synthesis, as well as a trustworthy device for catalyst testing and screening. However, compared with empty microchannels and macroscale packed beds with large particles inside, packed bed microreactors often produce a substantially larger pressure drop because (fine) particles restrict the size of flow pathways. It is thus crucial to conduct researches on pressure drop of packed bed microreactors, in order to optimize energy dissipation and gain knowledge about fluid flow as well as other relevant transport/reaction characteristics for further process optimization. In this research, the pressure drop behavior of single-phase (water or N2) flow in polymeric capillary microreactors packed with spherical glass beads of 60-1000 μm in size was studied firstly. The resulting bed porosities were measured, which could not be described by literature correlations for conventional packed beds satisfactorily. An empirical porosity correlation was proposed as a function of the microreactor to particle diameter ratio. The influence of particularly fluid flow rate, microreactor diameter and particle size on the obtained pressure drop data was revealed. This allows to examine the applicability of some typical literature pressure drop models for packed beds in microreactors, based on which further model improvement directions could be identified. Then, experiments of two-phase (typically N2-water) flow were performed in the above packed bed microreactors. The primary purpose is to elucidate the influence of the upstream inlet slug flow details, phasic flow velocity, two-phase flow ratio and packed bed properties on pressure drop. Based on the experimental results, the adequacy of the existing literature models was also examined. To gain a further understanding, some additional comparison with two-phase pressure drop in empty microreactors as well as single-phase pressure drop in the same packed beds will be performed. The findings of this research may provide useful insights in the design and operation of packed bed microreactors (e.g., optimized energy consumption and favorable operational window). Meanwhile, the results herein may illustrate to certain extent internal flow mechanisms inside packed bed microreactors, and give some guidelines for their promising use in highly efficient chemical synthesis or catalyst screening.

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Author: Sara Filipa Bentes Da Conceicao (Tu Delft)

Other Authors: Ana Somoza Tornos, TUDelft; Giljam Bierman, TUDelft

Title: **[I16] Solidification and Solute Redistribution During a Progressive Freeze Concentration Process -Theoretical Modeling and Experimental Validation**

Abstract: It is estimated that 30% of the CO2 emissions in the chemical industry originate from the fuel burnt in fired steam crackers [1]. Potentially it is possible to replace the fuel with renewable electricity and eliminate the 200 million tons of CO2 emitted anually. The objective of this project is to determine the best technology to supply heat to a cracker furnace, using electricity as the power source. A modern conventional furnace is used as reference case. The project proposes a furnace design that uses naphtha as feedstock and produces ethylene as primary product. The Netherlands is a suitable location for the implementation of the design, given its proximity to offshore wind energy sources and logistic routes. The processing capacity of a single unit is 168 kta of naphtha, and the ethylene yield is 50 kta (Figure 1). The battery limits for this project include the feed preheat and reaction section, conventionally called convection and radiation sections respectively. The process takes in a naphtha-steam mixture, preheats it to 600oC and delivers the reaction product at 850oC. The power requirement is 26 MW, which is provided using electricity. Five concepts are identified for heating: Plasma Torch, Hydrogen Furnace, Electric Resistive Heating, Molten Salts Reactor, and Rotodynamic Shockwave Reactor from which Electric Heating is selected as preferred technology. This concept has a high technology readiness level and can be used to achieve conventional capacities and yields (30%), with conventional residence times (0.1-0.5s). Two configurations of resistive heating are explored: conductive heating, in which the heating elements are in direct contact with the tube, and radiative heating, where the heating elements are mounted on the furnace wall (Figure 2). Flexibility to scale up, and opportunity to make the furnace compact, are advantages of conductive over radiative heating. However, further analysis on the coke formation using conductive heating must be performed, since it potentially leads to local temperature runaways. The proposed design is not radically different from conventional furnaces, as in both cases, naphtha is cracked inside tubes through which heat is transferred. However, conductive heating does not produce flue gas nor cause loss of energy with it. In addition, the preheating and reaction sections are now decoupled, thus simplifying the design. Under the current electricity mix [2], the electric furnace design does not reduce the CO2 emissions of naphtha cracking process, however, it is capable of saving on CO2 emission by means of a greener electricity mix.

[1]“Accelerating electrification with the ‘Cracker of the Future’. Repsol press release.” Sep.2021.
[2]M.Visser, “Renewable Energy in The Netherlands, Energy Academy Europe,” Jan. 2019.

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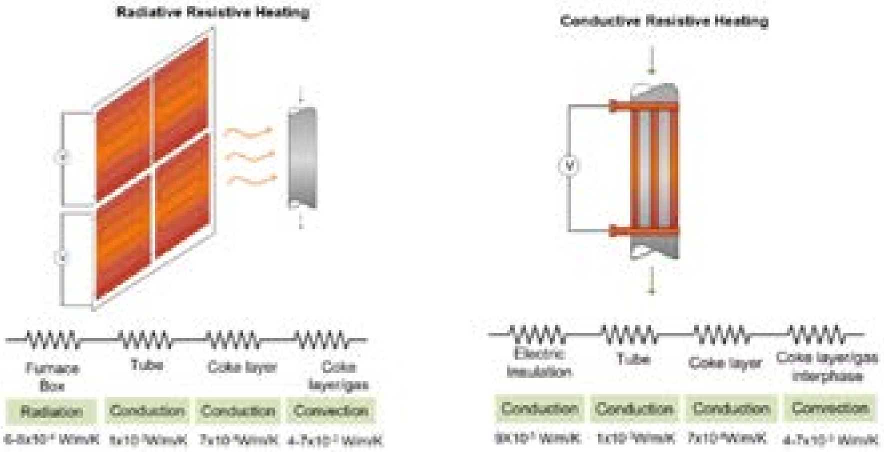

Figure 2: of the resistances to heat transfer in radiative and conductive heating configuration

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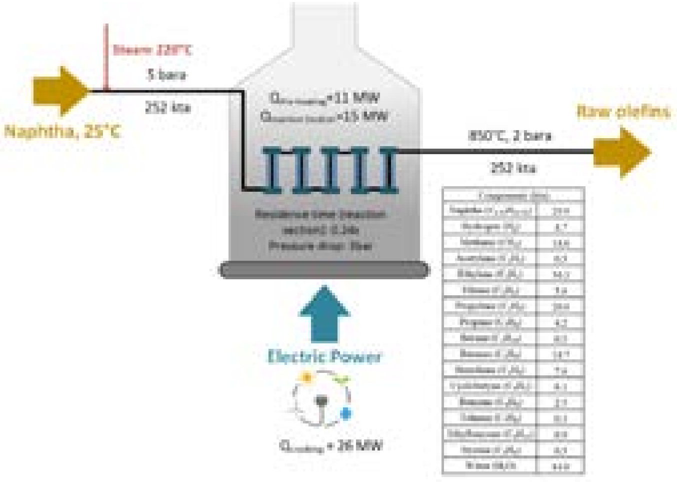

Figure 1: Input-output diagram of Naphtha cracking process

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Author: Claas Willem Visser (UTwente)

Other Authors: Olivier Nguon, UTwente; Jieke Jiang, UTwente; Kees Venner, UTwente

Title: **[L17] Fabricating multi-scale materials via in-air microfluidics**

Abstract: “Multi-scale materials that exhibit length scales between the molecular size and the part size are ubiquitous in nature, because diverse functionalities, efficient material use, and high performance can be integrated by tailoring across scales. However, fabricating these materials is challenging, as bulk processing technologies lack precision and microfluidic techniques lack throughput.

In this talk I will discuss methods based on liquid micro-jets that enable rapid fabrication of particles and 3D multiscale materials. The first part of the talk will discuss in-air microfluidics, a method to create micro-particles with controlled shape, size, morphology and composition. These particles are for example used in cell encapsulation, controlled release, and CO2 capture. The second part of the talk will address how the jetted droplets or bubbles are 3D-printed into functional multiscale materials. Here, the focus is on polymer foams and how we leveraged subtle mechanisms (oxygen inhibition) to control the open-to-closed cell transition and how the cell size and density are controlled. Applications including materials for tissue engineering and pressure sensors will be discussed.”

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Title: **[L18] Effect of gaseous contaminants on electrochemical CO2 reduction to C2+ products**

Abstract: Electrochemical conversion of CO2 into valuable fuels and chemicals has gained attention owing to the mild conditions applied and the possibility to integrate renewable energy sources to power the process. The CO2 feedstock for the electrochemical CO2 reduction reaction (CO2RR) could be obtained from various sources, such as from direct air capture (DAC) or from point sources such as the chemical industry or power plants. One of the major drawbacks of CO2 point sources is the presence of contaminants such as SO2, H2S, COS, NOx and other volatile organic compounds, which could be highly detrimental to the copper catalysts that drive the conversion of CO2 to C2+ products. These CO2 streams are typically cleaned using a series of amine-scrubbers and catalytic converters, however these are energy and capital intensive, making it desirable to study the effect of contaminants on the CO2RR and to determine the limits of each contaminant in order to derive an optimal feedstock cleaning procedure. In this work, we study the influence of various concentrations of sulfur-based gaseous contaminants such as SO2, H2S and COS in the CO2 feed on the selectivity, product distribution and catalyst stability during the CO2RR. A gas mixer is used to mix the selected contaminant with pure CO2 and produce concentrations such as 10000 ppm, 1000 ppm, 100 ppm and 10 ppm of the selected contaminant in CO2, which is then used as a feedstock for the CO2RR. Presence of SO2 above 100 ppm significantly suppresses the production of C2+ products and CO at -1.0 V vs RHE, however, at -1.2 V vs RHE, a significant suppression is not observed until above 1000 ppm of SO2. Since the onset potential for SO2 reduction is much lower than that of CO2RR, SO2 gets simultaneously reduced to S2- and deposits as CuS on the surface of the Cu catalyst, which ultimately blocks the active sites for the CO2RR. The main products observed under the suppressed conditions are hydrogen, formate and small amounts of methane. In the case of H2S, the detrimental limits are even lower than that of SO2, where a significant suppression of C2+ products is observed even at 10 ppm of H2S at -1.0 V vs RHE. While at -1.2 V vs RHE, a significant suppression of C2+ products is not observed until above 100 ppm of H2S. COS proved to be the most detrimental to copper catalyst with even 10 ppm of COS suppressing the production of C2+ products at both -1.0 V and -1.2 V vs RHE. Long recovery experiments show that it takes at least 4 hours of purging with pure CO2 and a constant voltage supply to (partially) regenerate the copper catalyst after exposure to 1 h of 10000 ppm of SO2/H2S/COS, making the continuous operation of the CO2RR plant difficult in the presence of these contaminants.

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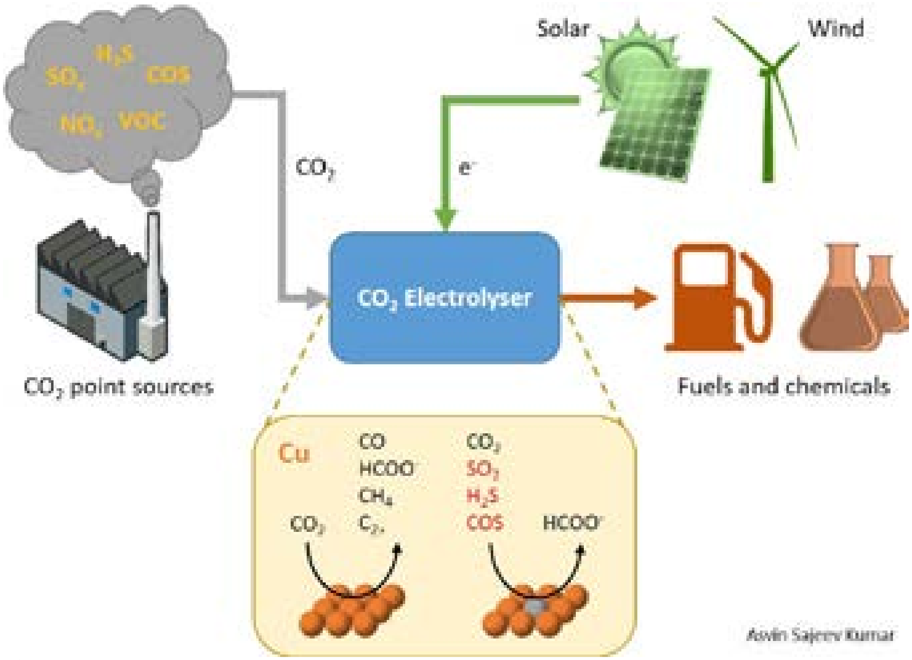

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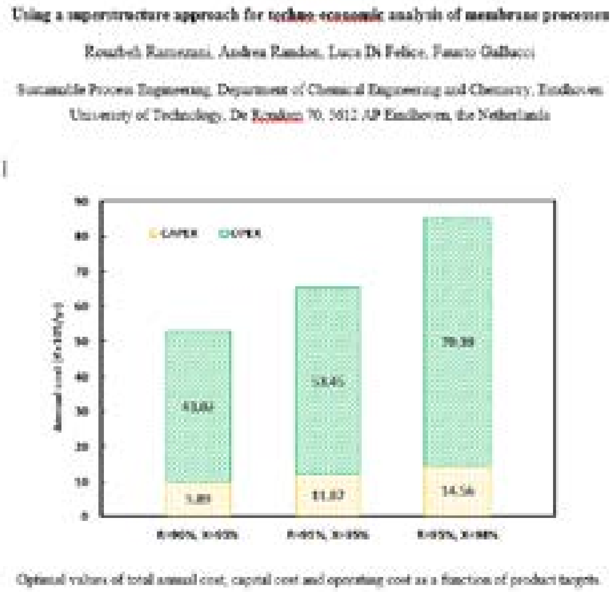
Author: Rouzbeh Ramezani (TU/e)
Other Authors: Andrea Randon, Luca Di Felice, Fausto Gallucci

Title: **[L19] Using a superstructure approach for techno-economic analysis of membrane processes**

Abstract: The alarming increase in global CO2 emissions warrants the acceleration of CO2 capture technologies. Membrane technology has been regarded as a potential promising separation technology due to its low energy consumption and low carbon footprint. While most scientific research is focused on developing novel materials for this application, it is the process design of the membrane operations that is much more critical in reducing capture costs. A superstructure membrane design is proposed here to study the implementation of a multi-stage membrane approach for CO2 separation from different industrial sources of CO2 emission by process simulation tools. A bio-based membrane with high CO2 permeance, membrane CO2/N2 selectivity of 25 and CO2/CH4 selectivity of 8 is used. Three major sweetening processes are considered such as post-combustion CO2 capture, biogas upgrading, and natural gas sweetening. A rigorous simulation-based optimization model is applied to determine the most efficient membrane strategy from a gas processing cost, specific energy consumption, and membrane area point of view. By proposing a superstructure-based model, the number of stages, recycle options, use of feed compression and/or permeate vacuum, and operating conditions are simultaneously optimized to minimize the total annual cost. The carbon capture cost and energy consumption of the optimal cases were reported according to the economic evaluation. In detail, the effect of feed and permeate pressure, membrane selectivity, product purity, and recovery on CAPEX, OPEX, total membrane area, net power demand, and gas separation cost are examined.



Using a superstructure approach for techno-economic analysis of membrane processes

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Optimal values of total annual cost, capital cost and operating cost as a function of product targets.

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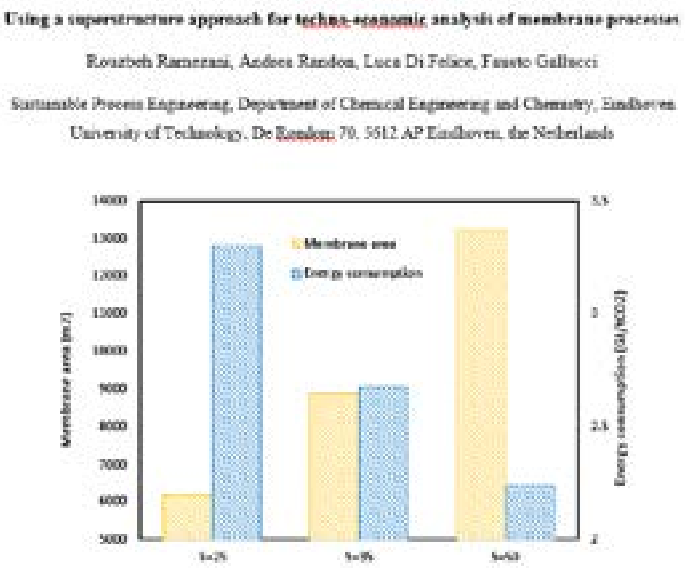

Using a superstructure approach for techno-economic analysis of membrane processes

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Title: **[L20] Membrane performance and mass transfer with adjusting solution pH and ionic strength during fractionating a fish protein hydrolysate.**

Abstract: Pressure-driven membrane processes are promising to fractionate bioactive peptides from protein hydrolysates as most bioactivities are present with peptides smaller than 4 kDa in size. Many researchers have proposed that membrane processes could be used for this purpose in dairy-based sources. Recently, it was reported that fish protein hydrolysates contain peptides with various bioactivities such as antioxidant, antihypertensive, and Angiotensin-I-Converting Enzyme (ACE) inhibiting action. This work focuses on applying spiral wound membranes for fractionating a fish protein hydrolysate to study the factors affecting the separation process and mass transfer mechanism. A commercial fish protein hydrolysate (Prolastin®) was treated using three polyether sulfones (PES) and a polyamide-TFC (PA) spiral wound membranes with different MWCOs on a pilot scale. Experiments were done at various solution pH (5 and 8), with and without addition of NaCl. The membrane performance was evaluated in terms of permeate flux and retention. The highest permeate flux was obtained at the alkaline condition for all PES membranes, regardless of adding salt. In addition, the presence of NaCl enhanced the permeate flux but diminished the membrane retention. The apparent MWCO of each membrane could be altered by changing the solution pH and salt concentration.

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Title: **[L21] Dry fractionation for sustainable recovery of protein enriched ingredients: A focus on powder properties**

Abstract: Protein ingredients from legumes are of major interest for both research and commercial purposes. Dry fractionation (i.e. milling, and subsequent air classification or electrostatic separation) can be used to produce protein, starch and fibre-rich fractions with a clean label and lower environmental impact than traditional wet fractionation. The native states of protein and starch are preserved upon dry fractionation and allows making of ingredient fractions that exhibit unique functional properties. High relative humidity (RH) upon storage and higher oil contents can negatively influence the milling and dry fractionation behaviour of legumes, which would be related to reduced particle flowability. Our focus is thus to establish optimal dry fractionation of legume flours by unravelling the effect of RH and oil content on powder properties (particle- size, dispersibility and flowability) and process performance (milling, air classification and/or electrostatic separation) (Figure 1). Soybean oil was mechanically removed prior to fine milling to evaluate the effect of oil content on milling performance and particle size and dispersibility. Furthermore, we varied the humidity of the processing air and storage environment between 30% and 70% for milling and air classification of yellow pea (0.8 %DM oil) and chickpea (5.2 %DM oil). We used a pressure titration to evaluate the particle size and dispersibility and we adopted a dynamic measurement sequence based on a descending and ascending movement of a rotating blade to assess the flowability of the produced and stored flours. We found that a higher oil content limits milling to smaller particles and results in less dispersible fine particles below 10 µm (i.e. protein bodies), which might hamper further separation. A change in the RH during milling and air classification does not significantly affect milling- and separation performance in the range of 30-70% RH. However, storage (1 week) of chickpea flour at a humidity of 70% decreased the air classification performance due to a lower particle dispersibility and flowability. Thus, a relative humidity above 70% should be prevented to perform robust air classification. Improving the particle dispersibility and flowability of legume flours by de-oiling or by keeping the RH below 70% improves milling and dry separation of legumes. This enables a more effective use of the biomass with a reduced environmental impact

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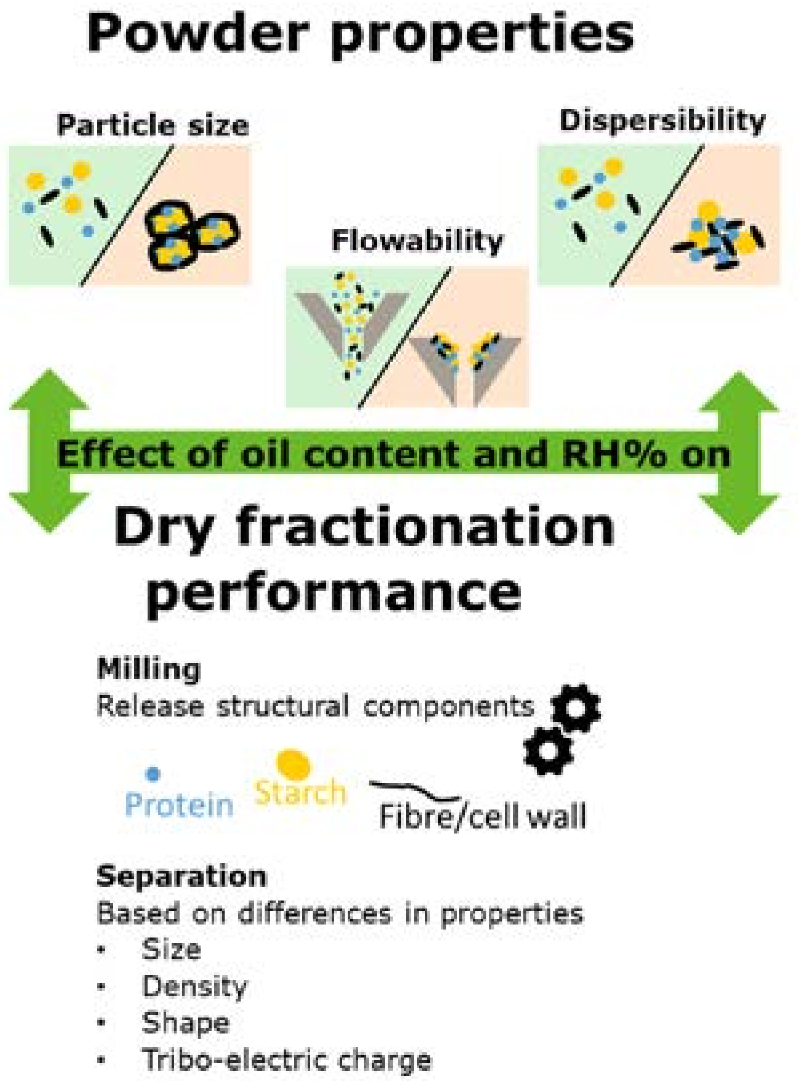

Figure 1: Visualisation of our research on powder properties and dry fractionation, where light green illustrates favourable powder properties and light orange unfavourable powder properties for dry fractionation (milling + separation).

NPS2023 Figure 1 Regina Politiek.png

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Author: Hilda Lucy Nyamburana (WUR)

Other Authors: Anja E.M. Janssen, Wageningen University & Research; Remko Boom, Wageningen University & Research; Albert van der Padt, Wageningen University & Research

Title:

[L22] Prediction of Permeate Flux and Rejection during Microfiltration of Skim Milk at Low Temperature Using a Geometric Model

Abstract:

“In the dairy industry, crossflow microfiltration is one of the major processes used during fractionation of milk proteins. Currently, there is a rise in the use of polymeric membranes in spiral wound configuration at lower temperatures of 10°C. The performance indicators of these membranes during fractionation process are both rejection of different milk proteins and the permeate flux obtained. These factors are determined using membrane properties such as membrane configuration and pore sizes as well as process conditions namely temperature and applied pressure. Through experiments, optimum membrane properties and process conditions can be identified based on the desired end product. However, this process is tedious and time consuming. Therefore, modelling of protein rejection and flux behavior during milk protein fractionation is a necessity. For this, comprehensive understanding of the behavior of the concentration polarization layer formed during filtration is required. This layer influences the flux and retention behavior depending on its complexity. Properties of this layer can be incorporated to create a model of permeate flux and retention of milk proteins which has not been addressed. To address this gap, a geometric model for the build-up of retention for dissolved proteins by accumulation of casein micelles in the concentration polarization layer is developed. For this, casein micelles are assumed to be soft deformable spheres and when in contact there are interstitial pores between them that are relatively large and can allow whey protein to pass through. Before, reaching the limiting transmembrane pressure, the concentration polarization layer has not fully formed and micelles are still fluid and can move back to bulk. As soon as the volume fraction reaches an approximate value of 0.36 due to application of pressure, the concentration polarization starts to form. Due to the pressure applied, the micelles start deforming reducing the interstitial pores and the measure for this deformability is the interfacial tension. Using the size of the protein, size of interstitial pores, interfacial tension and pressure over the concentration polarization layer, rejection can be determined using the Ferry equation (Cherkasov & Polotsky, 1996). Moreover, the flux can be determined based on the membrane and concentration polarization layer resistance, milk viscosity, mass transfer and transmembrane pressure (Beckman & Barbano, 2013; Hartinger et al., 2019; Lawrence et al., 2008). When we incorporate this in a simple numerical model, we can predict the flux and the retention of the protein. These predictions are coupled with experimental results. In future this predictive model can be combined with shear induced model.

References: Beckman, S. L., & Barbano, D. M. (2013). | Cherkasov, A. N., & Polotsky, A. E. (1996). |Hartinger, M., Heidebrecht, H. J., Schiffer, S., Dumpler, J., & Kulozik, U. (2019). | Lawrence, N. D., Kentish, S. E., O’Connor, A. J., Barber, A. R., & Stevens, G. W. (2008).

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Author: Kaustub Singh (TU Delft)
Other Authors: David Vermaas, TU Delft

Title: **[L23] Evaporative crystallization of sessile droplets using electrowetting**

Abstract: An increasing focus on the use of renewable energy has consequently brought attention on the state-of-the-art of energy storage. Systems with scalable and decoupled power and energy, such as flow batteries, will become essential in the overall energy transition for long-duration energy storage. Within flow batteries, acid-base flow batteries (ABFBs) offer a tremendous opportunity to store energy in acids and bases, made by splitting abundantly available and benign salts (e.g. NaCl), for long duration. While the ABFB is in pilot stage, several aspects about its long term performance require attention and further development. One such point of investigation is the bipolar membrane (BPM), the heart of the ABFB technology, illustrated in Figure 1. Flowing acid and base streams on either side of the BPM develops a potential difference over it, which is harnessed by current to generate power and thus, extract energy from the said acid and base streams. Given the crucial role of BPMs in ABFB, it is imperative to understand the transport of ions through it since any unwanted flux of ions across the membrane shall immediately reduce the energy efficiency and contaminate the acid and the base solutions, jeopardizing long term battery operation. Here, we elucidate one such unwanted ion transport through the BPM: the crossover of co-ions between the acid, salt, and base. We show, from 12 hr. cycling experiments, the contamination of the base stream (NaOH) with the co-ion (Cl-) from the acid stream (HCl), flowing on the other side of the BPM. We find that the gradual increase of Cl- in the base is linked to the state of charge of the ABFB. Comparing the crossover in different state of charge allows to quantify co-ion transport in the individual membranes during operation of the flow battery. Figure 2 presents this comparison between a charged and a discharged battery. We hypothesize on the reason of this crossover and reflect on the mitigation strategies to prolong the cycling time of the ABFB.

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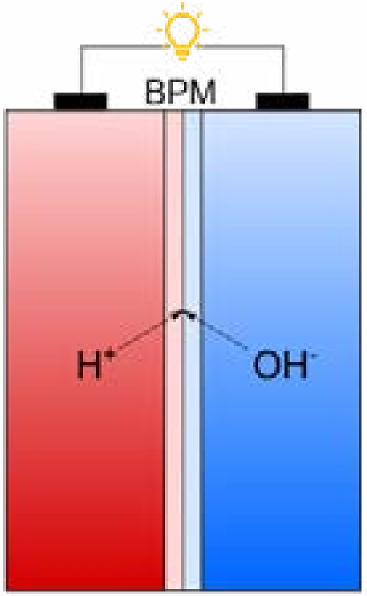

Figure 1: Bipolar membrane, separating acid and base streams and generating potential difference.

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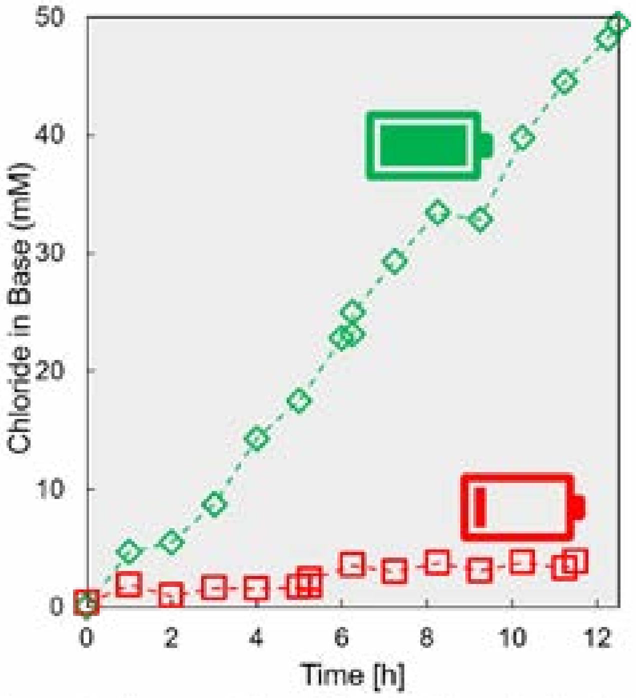

Figure 2 : Accumulation of Chloride ions in the base compartment as a function of operation time for a charged (green) and a discharged (red) ABFB.

000041-S-figure-2-base-contamination.png

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Author: Marrit van der Wal (TU/e)

Other Authors: Prof. Dr. Ir. Kitty Nijmeijer, TU/e; Dr. Ing. Zandrie Borneman, TU/e

Title: **[L24] Dynamic ammonium retention in membrane processes for nutrient separation from manure**

Abstract: The agricultural sector aims to valorize manure by producing separate fractions for further use in precision fertilization while limiting nitrogen and CO_2 emissions. To do so, this often involves the production of biogas by co-digestion of the manure, followed by several mechanical and membrane separation steps of the remaining digestate to produce nutrient-rich fractions [1]. Such separate nutrient-rich fractions, containing phosphorus, nitrogen or potassium, allow tailoring the nutrient ratio per crop and season for precision fertilization, reducing the need for artificial fertilizer. After the mechanical separation of the digestate into a solid phosphorous-containing fraction and a liquid fraction containing nitrogen and potassium, the liquid fraction is further treated. Especially, the nitrogen and the potassium present in this liquid fraction are difficult to separate. Nitrogen is mainly present in the form of ammonium ions (NH_4^+) which have a similar charge valency, ionic radius and hydration shell as potassium. However, NH_4^+ is in equilibrium with NH_3 and where NH_4^+ is mostly retained by the membrane, NH_3 can easily permeate the membrane. As the NH_4^+/NH_3 equilibrium is very sensitive to pH, the pH can be used to tune the separation of nitrogen relative to potassium species. At a high pH, the acid-base equilibrium shifts towards NH_3 while at a low pH NH_4^+ is mostly present. So that at high pH, the feed mixture contains mostly K^+, which is retained, and neutral NH_3¬ molecules that permeate the membrane as shown in Figure 1 [2]. In this research, we investigate this dynamic ammonium retention of nanofiltration and reverse osmosis membranes by varying the pH of the feed streams in order to tune the nitrogen permeation using artificial K^+/NH_4^+ feed mixtures as well as real manure feeds at different pH values separated using a stirred cell over a pressure range. The results show increased nitrogen permeations through the membranes at high pH values thus reaching low nitrogen retention values of approximately 30%. Moreover, at these high pH values the retention of potassium remains high at approximately 90%. This resulted in significant separation of N from K resulting in a fraction increased in nitrogen concentration and a fraction rich in potassium to be used for precision fertilization.

[1] Velthof, G.L. (2015) Alterra Report 2650.
[2] Masse, L. (2008) Journal of Membrane Science

Acknowledgement: This publication is part of the project “No Time to Waste” with project number ENPPS.LIFT.019.018 of the research programme LIFT which is (partly) financed by the Dutch Research Council (NWO).

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Pre-filtered digestate at high pH

Figure 1: A schematic overview of the pH influence on the retention or permeation of potassium and nitrogen species through an NF or RO membrane.

Marrit van der Wal

000054-Q-2301231-schematic-overview-of-the-ph-influence-on-n-k-separation.tif

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Author: Mahsa Gholami (UTwente)

Other Authors: Boelo Schuur, University of Twente; Jochem M. Tijburg, University of Twente

Title: **[L25] Study of organic solvents in the extraction of lignin and furanics from deep eutectic**

Abstract:

Extracting and purifying lignin from wood without compromising cellulose quality too much is a challenging process. Lactic acid: choline chloride is a deep eutectic solvent (DES) that has been identified as acceptable delignification solvent, producing lignin, hemicellulose and smaller molecules as by-products to the cellulose. Hemicellulose is partly transformed into furanic compounds (e.g., furfural and 5-HMF). While the larger lignin can be obtained by water precipitation from DES, smaller lignin molecules and furanics can be recovered by liquid-liquid extraction (LLX), either directly or after first precipitating the larger lignin. The presence of water in the DES after water precipitation reduced the mutual miscibility with the solvents, and allowed the use of a wider range of solvents in the LLX process than when LLX was applied directly after cooking. In the precipitation stage of the process, all the larger molecular weight lignin molecules (Mw>5000 Da) can be recovered when adding at least 3.5 [g/g] water to DES- black liquor. For the combined precipitation+LLX study, also solvents that were previously rejected in the screening study were investigated again, and guaiacol was found as suitable alternative to the previously published 2-methyltetrahedrofuran (2-MTHF). In addition, here we report the use of 2,2,5,5-Tetramethyl oxolane (TMO), a recent addition to the palette of (potentially) bio-based solvents. The distribution coefficients of smaller lignin molecules and furanics in LLX with guaiacol, TMO and 2-MTHF-based extractions were compared, revealing that smaller lignin molecules (500-5000 Da) can be recovered with a reasonable distribution coefficient by 2-MTHF and guaiacol. Furfural shows distribution coefficients of at least 1.27 for all three solvents. TMO is least effective for 5-HMF extraction, with distribution coefficients around 0.5. However guaiacol and TMO both have a significantly lower lactic acid leaching. This makes them a potential alternative for 2-MTHF in this technique, especially when less water is required for the precipitation step.

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Author: Burak Eral (TU Delft)

Other Authors: Nagaraj Nagalingam; Aswin Raghunathan;Vikram Korede; Christian Poelma; Carlas S. Smith; Remco Hartkamp; Johan T. Padding; Huseyin Burak Eral

Title: **[L26] Laser-Induced Cavitation for Controlling Crystallization from Solution**

Abstract: We demonstrate that a cavitation bubble initiated by a Nd:YAG laser pulse below breakdown threshold induces crystallization from supersaturated aqueous solutions with supersaturation and laser-energy dependent nucleation kinetics. Combining high-speed video microscopy and simulations, we argue that a competition between the dissipation of absorbed laser energy as latent and sensible heat dictates the solvent evaporation rate and creates a momentary supersaturation peak at the vapor-liquid interface. The number and morphology of crystals correlate to the characteristics of the simulated supersaturation peak.

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Author: Chencong Ruan (RUG)

Other Authors: Jun Yue, University of Groningen

Title:

[L27] Reactive extraction-promoted 5-hydroxymethylfurfural production in deep eutectic solvents in batch reactors and microreactors

Abstract:

The catalytic transformation of biomass-derived carbohydrates (e.g., cellulose and hexose) to platform chemicals such as 5-hydroxymethylfurfural (HMF) has attracted vast attention over recent years, since HMF is a versatile chemical to manufacture valuable bio-based chemicals, fuels and functional materials. Deep eutectic solvents (DESs) as a novel and green solvent have been increasingly used as the reaction medium for HMF production, because of the advantages of suppressing side reactions and synergistically catalytic effect. Reactive extraction is considered as a potential and efficient process intensification technology for HMF synthesis, where a biphasic system is built to in-situ extract HMF from the reaction phase to an extraction phase thus suppressing HMF-involved side reactions (Fig.1). Generally, organic solvents like methyl isobutyl ketone (MIBK) are used as the extraction agent that has a good extraction capability to HMF. In the concept of reactor design, continuous flow microreactors hold numerous benefits over conventional (batch) reactors, such as high mass and heat transfer rates (resulting from large specific surface areas) and precise control over reaction conditions, thus providing a compelling opportunity for developing more efficient catalytic processes of HMF production. In this work, DESs composed of choline chloride (ChCl) and ethylene glycol (EG) at different molar ratios (1:2, 1:3 and 1:4; labeled as [ChCl:2EG], [ChCl:3EG], [ChCl:4EG], respectively) were applied to build a DES-MIBK biphasic system for the synthesis of HMF from fructose in both batch reactors and microreactors. Firstly, the conversion of fructose over HCl catalyst in monophasic and biphasic solvent systems in batch reactors was studied, in order to obtain optimized reaction and operation conditions. In monophasic system, the effects of temperature, batch time, HCl loading and DES composition (i.e., ChCl-to-EG molar ratio) on the fructose conversion and HMF yield were revealed. The application of biphasic system significantly boosts the HMF yield, e.g., increasing from 48% to 63% at 80 oC, 5 mol% of HCl loading, and a phasic volume ratio of 3:1 (MIBK:DES) in [ChCl:3EG]. Based on the optimized results in batch reactors, experiments were performed in capillary microreactors under slug flow operation to explore the potential of combining microreactor technology with DES-MIBK biphasic system for the continuous production of HMF. Microreactors were shown to rapidly heat up the feedstock to the reaction temperature (i.e., within ca. 40 s), while it took 5 min in batch. As a result, microreactors afford a higher conversion rate, e.g., a fructose conversion of ca. 58% was achieved within 2 min in microreactors in comparison with 36% in batch. However, the highest HMF yield (61%) in microreactors is a bit lower than that measured in batch reactors (63%). This is ascribed to a slight mass transfer limitation in microreactors, thus further improvement is needed.

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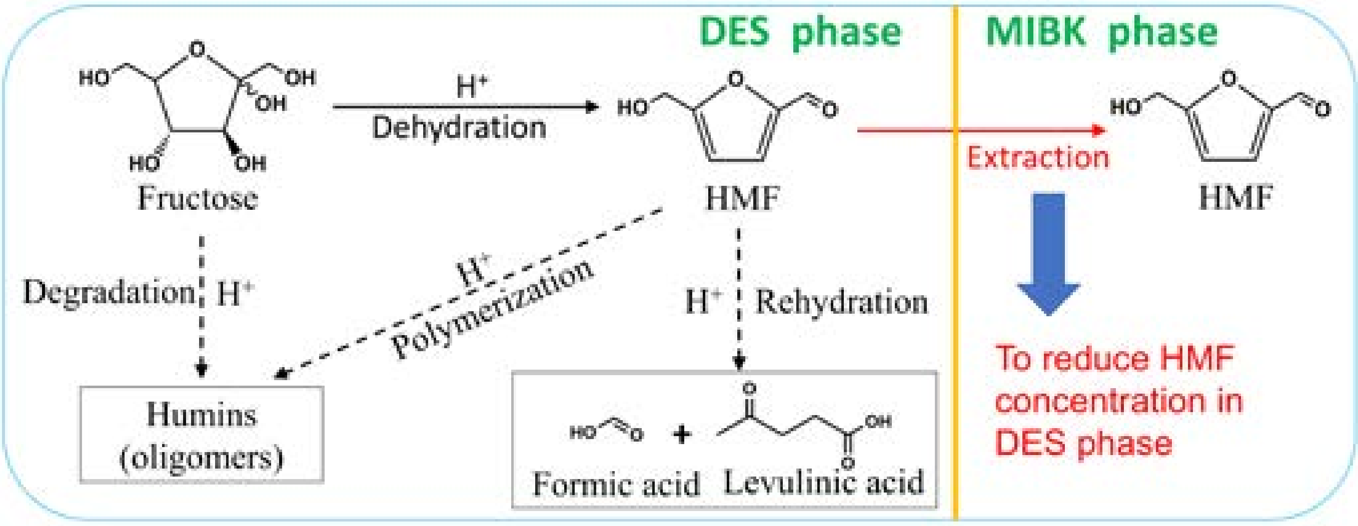

000021-Q-fig.-1.-scheme-for-hmf-production-from-fructose-in-the-des-mibk-biphasic-system.tif

Author: Tim van Schagen (UTwente)

Other Authors: Wim Brilman, University of Twente

Title: **[L28] LOGIC 2.0: Towards a natural convection driven, autothermal and condensing methanol reactor**

Abstract: In the past three years the second version of the Liquid-Out, Gas-In Concept (LOGIC) methanol reactor was designed, modelled, built and tested at the University of Twente in collaboration with project partners. In the reactor, CO2 and H2 are converted to methanol and water over a commercial Cu/ZnO/Al2O3 catalyst. The reactor contains an internal condenser to remove the water and methanol as liquids, bypassing the reaction's equilibrium limitations. By placing the cool condenser above the hot catalyst bed, internal gas recycling is achieved by natural convection. Finally, internal heat integration between the hot catalyst outlet stream and the cold gas recycle stream from the condenser is applied to achieve autothermal operation. In this presentation and overview will be given of the main achievements in the LOGIC 2.0 project. For the conceptual design of the reactor, a steady-state flowsheet model with custom thermodynamics engine was developed to compare different design options and reactor scales. After the basic reactor design was chosen, it was modelled in detail using a dynamic 1D CFD model, which includes the effects of natural convection, chemical reactions and heat transfer. With this model, the detailed design parameters were chosen based on the results of sensitivity analyses. It was found that the reactor height, catalyst bed length, catalyst bed inlet temperature and system pressure are the most important system parameters. The dynamics of the system were also investigated to assess start-up and shut-down effects. A large uncertainty of the design was the heat transfer behaviour in the heat integration zone of the reactor. To investigate this, a 2D CFD model was developed and used to determine the heat transfer coefficient in the heat integration zone under varying conditions. The effect of local natural convection effects was found to have a large impact, leading to a non-classical flow profile in the system. Finally, the reactor was built and tested so that the experimental results can be used to validate the modelling work.

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Author: Lola Azancot Luque (UTwente)
Other Authors: Leon Lefferts, University of Twente

Title: **[L29] Catalyst deactivation in methanol synthesis**

Abstract: Methanol is one of the most interesting products synthesised from CO2 by hydrogenation, contributing to decarbonization via CO2 capture and utilisation. Methanol is an intermediate for synthesis of multiple chemicals, such as methyl tertiary-butyl ether (MTBE), dimethyl ether (DME), olefins and fuels. This is reflected in increasing production from 2009 (53.9 Mt) to 98 Mt in 2019 and is expected to raise to 500 Mt in 2050, according to International Renewable Energy Agency (IRNA) Transforming Energy Scenario.

Methanol synthesis from CO2 (Eq. 1) is an exothermic reaction requiring high-pressure and low temperature, according to Le Châtelier´s principle, shifting the thermodynamic equilibria to achieve high CO2 conversion and methanol selectivity. Low temperature is also required to minimize CO formation via the reverse water gas shift (rWGS) reaction (Eq. 2).

$$\mathrm{CO2 + 3H2} \leftrightarrow \mathrm{CH3OH + H2O} \quad \Delta H\ 298\ \mathrm{K} = -49.5\ \mathrm{kJ\ mol\text{-}1} \quad \text{(Eq. 1)}$$
$$\mathrm{CO2 + H2} \leftrightarrow \mathrm{CO + H2O} \quad \Delta H\ 298\ \mathrm{K} = 41.2\ \mathrm{kJ\ mol\text{-}1} \quad \text{(Eq. 2)}$$

The Cu/ZnO/Al2O3 catalyst for methanol synthesis is the catalyst par excellence, introduced 50 years ago for methanol synthesis from syngas. It is still under debate what the active site exactly is and how the key components, i.e. Cu and ZnO, participate in the reaction. It is becoming increasingly clear that the interaction between these components changes with reduction pre-treatment, reaction conditions and time-on-stream. Diverse hypotheses about the catalyst deactivation in industrial conditions have been suggested, such as, that the deactivation could be responsible for the ZnO mobility, Cu and ZnO sintering accelerated by water, brass (Cu-Zn alloy) formation or oxidation of Cu. However, a deep understanding of these structural changes is still missing, encouraging further research.

Our work is focused on understanding the structural properties, from activation to reaction, to obtain a clear and extended picture of Cu and ZnO synergy and their possible changes under reaction conditions. Better understanding of catalyst deactivation and identification of the cause of deactivation are essential to increase trust in sufficient lifetime of the catalysts, indispensable for successful industrial application.

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Author: Tingting Wang (RUG)

Other Authors: Thom Meeuwes, University of Groningen; Jun Yue, University of Groningen

Title:

[L30] Experimental study of doplet-side mass transfer in slug flow capillary microreactors

Abstract:

Liquid-liquid slug flow in microreactors has found promising uses in solvent extraction and biphasic reactions, due to among others its high mass transfer rates, precise flow controllability and remarkable efficiency enhacement. The fundamental knowledge on mass transfer in slug flow is necessary for an in-depth understanding into the process performance and its optimization. Up to now, rather limited systematical analyses are available focusing on the specific transport mechanism. In our previous work of Susanti et al. [1], a slug flow mass transfer model according to the penetration theory has been developed based on the experimental extraction of acetanilide from water to n-octanol. In the model, droplets and slugs are simply treated both as stagnant fluids. As a result, an additional fitting parameter (2.6) has to be included to account for the enhancement of internal recirculation at a 1:1 aqueous to organic flow ratio. Herein, the applicability of this model needs to be examined in wider flow conditions (e.g., in terms of different flow ratios) and more reaction systems (e.g., in terms of different individual mass transfer resistance). In this work, experiments on the extraction of ethyl acetate have been studied as a model system in the polytetrafluoroethylene microreactor (i.e., involving only aqueous-side mass transfer resistance). The aqueous phase presented as the droplet in the generated slug flow pattern. The formed slugs and droplets were separated at the microreactor outlet by using a phase spitter according to the wettability difference. Then, the outlet concentration of ethyl acetate in the aqueous phase was analyzed with a UV–visible spectrometer, based on which the droplet-side mass transfer coefficient (kL) could be calculated.
From the experiments, the measured variation of slug and droplet lengths with flow ratio was analyzed, which allows the estimation of interfacial area (a) for mass transfer. Then, the influence of flow ratio and residence time on the mass transfer coefficient in the droplet was discussed. It was found that the mass transfer coefficient decreased at longer residence times, which is qualitatively in line with the model prediction of Susanti et al. [1]. However, the additional fitting parameter to describe the contribution of internal circulation in the model was found dependent on the flow ratio. The reasons for this dependence will be discussed based on the recirculation and diffusion patterns inside droplets of different lengths.

[1] Susanti, Winkelman J G M, Schuur B, et al. Lactic Acid Extraction and Mass Transfer Characteristics in Slug Flow Capillary Microreactors. Industrial & Engineering Chemistry Research, 2016, 55: 4691-4702.

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Author: Cristina García Llamas (TU/e)

Other Authors: J.A.M. (Hans) Kuipers, TU/e; K.A. (Kay) Buist, TU/e; M.W. (Maike) Baltussen, TU/e

Title: **[L31] Numerical investigation of the primary break-up of a jet for laminar and turbulent conditions**

Abstract: Primary atomization is a process where a liquid stream transforms into an array of ligaments and droplets. Understanding the phenomena governing the primary break-up of a jet is of foremost importance for many industrial applications.
To investigate the physical mechanisms influencing the break-up of a jet, Direct Numerical Simulations (DNS) are performed for different break-up regimes (i.e., Rayleigh regime, second-wind induced regime and turbulent Rayleigh regime).
To capture the deformation and topological changes of the gas-liquid interface of the jet, the Local Front Reconstruction Method (LFRM) is used. The numerically obtained break-up lengths and deformations of the jets are compared to experiments and literature. The results show that LFRM accurately describes the break-up lengths and droplet sizes in the laminar regime. In addition, LFRM captures the abrupt deformations on the interface surface as well as the merging and break-up of the formed droplets in the turbulence dominated regime.

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Author: Arnab Chaudhuri (TU Delft)

Other Authors: Timothy Noel, University of Amsterdam; John van der Schaaf, TU/e

Title: **[L32] Photochemical Transformations using the Rotor-Stator Spinning Disc Reactor**

Abstract: Photochemical transformations have witnessed a remarkable growth of attention in the past decade. This has been fueled by the popularity of photoredox catalysis and the technological progress in energy-efficient light sources. Despite the growing attention towards this field, the scaling of these photon-induced processes remains a daunting challenge, often discouraging their implementation in the production of fine chemicals and pharmaceuticals. To address this issue, here, we report the development of a novel reactor, the photo rotor-stator spinning disk reactor. The operating principle of this device relies on the generation of a high amount of turbulence in a cavity of a few millimeters with a rapidly rotating disk (Fig1 I.). We have demonstrated the efficacy of the rotor-stator spinning disk reactor for the intensification of photochemistry by studying both a gas-liquid reaction [1] as well as a gas-solid-liquid reaction[2]. The gas-liquid reaction involved [4 + 2] cycloaddition between α-terpinene and singlet oxygen to form the drug, ascaridole. Due to improvements in mass transfer, brought about through the generation of turbulence from the rotation of the disk, the conversion and selectivity increased from 37% to 97% and 75% to 90% respectively with an increase of rotation speed from 100 to 2000 RPM. We were able to obtain throughputs of over 1 kg/day (270 mmol/h) under visible light irradiation (Fig 1 II.). For the gas-liquid-solid reaction we investigated the photodegradation of methylene blue, with TiO2 as a slurry catalyst. This reaction system has direct application for dye waste water treatment. The use of the RS-SDR was vital for improving the dispersion of the slurry catalyst as well as for the improvement of the irradiation profile in the reactor. These results illustrate the potential of the rotor-stator spinning disk reactor for the intensification of photochemical processes and can perhaps help pave the way to continuous processes in the fine chemicals and pharmaceutical industry.

References

1. Chaudhuri, Arnab, et al. “”Process intensification of a photochemical oxidation reaction using a Rotor-Stator Spinning Disk Reactor: A strategy for scale up.”” Chemical Engineering Journal 400 (2020): 125875.
2. Chaudhuri, Arnab, et al. “”Scale-Up of a Heterogeneous Photocatalytic Degradation Using a Photochemical Rotor–Stator Spinning Disk Reactor.”” Organic process research & development 26.4 (2022): 1279-1288.”

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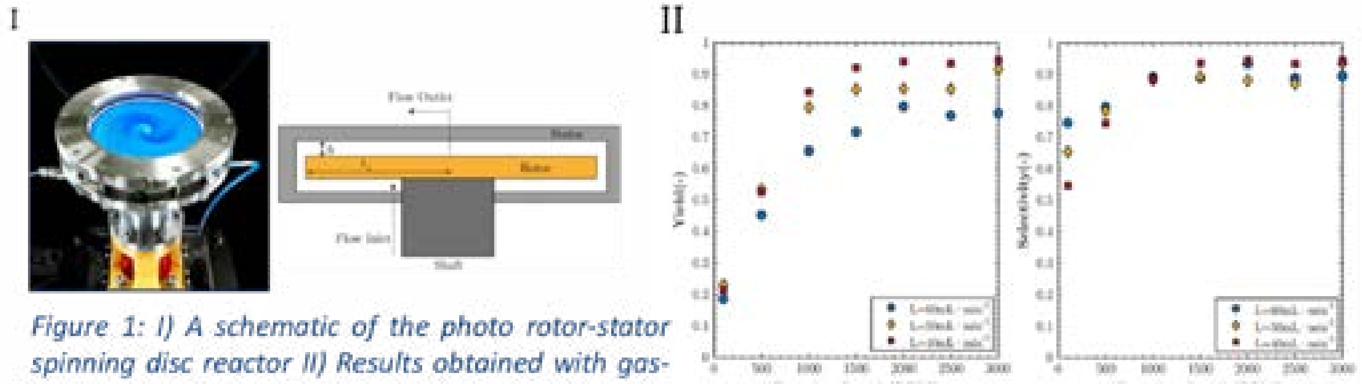

Figure 1: I) A schematic of the photo rotor-stator spinning disc reactor II) Results obtained with gas-liquid singlet oxygen reaction of α-terpinene in the photo rotor-stator spinning disc reactor

000092-Q-nps-figure-arnab-chaudhuri.png

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Author: Kun Xin (TU/e)

Other Authors: Jurriaan Boon, TNO; Eric van Dijk, TNO; Paul Cobden, TNO; Martin van Sint Annaland,TU/e

Title: **[L33] Stability of potassium-promoted hydrotalcite for CO2 capture under different adsorption/desorption cycles**

Abstract: Hydrotalcite based sorbents have been widely used for CO2 capture, especially in the sorption enhanced water gas shift (SEWGS) process. While the stability of this material under multiple repetitive adsorption/desorption cycles are still unclear. In this work, the effects of various long-term operating cycles such as CO2 adsorption → steam flush, CO2&H2O co-adsorption → N2 flushing, CO2&H2O co-adsorption → steam purge, steam adsorption → N2 flushing, and also CO2 adsorption → N2 flushing et al. on CO2 capacity and morphological change of potassium-promoted hydrotalcite based sorbents were investigated, combining thermogravimetric analyses and various techniques. When the sorbent is exposed to different working cycles, there are hardly no changes in SEM images and SEM technique is not suitable to investigate the morphological changes. Apart from the sorbent pores turn into larger sizes after different treatments, the BET surface areas keep slightly changed. By combining EDX technique and ICP-MS analysis, we find K2CO3 is dispersing everywhere on the sorbent. The investigated potassium-promoted hydrotalcite is a heterogeneous sorbent (from EDX mapping) and XRD technique is selected to identify the change of K2CO3 dispersion on the sorbents after different treatments.The studied sorbent loses cyclic capacity within the cycles of CO2 adsorption/N2 flushing, due to the slow desorption rate of CO2 during N2 flushing. Heat treatment at 600 °C can only partially restore the sorption capacity of 0.25 mg/g. Besides, early exposure of the potassium-promoted hydrotalcite with steam purge/N2 flushing cycles will result in a capacity loss of 0.5 mg/g. The CO2 adsorption mechanism keeps the same after the sorbent is exposed to steam purge/N2 flushing cycles. The decreased number of adsorption sites which is because of K2CO3 aggregation from the sorbent (XRD analyses) results in the loss in capacity. While if the sorbent has already been used after 80 cycles of CO2 adsorption/N2 flushing, cycles of steam purge/N2 flushing will help restore the sorbent capacity. The reconstruction of the sorbent under air, N2 and other gas mixtures was also investigated. Further, the potassium-promoted hydrotalcite is stable in view of both structure and sorption capacity over cycles of CO2 adsorption → steam flush, CO2&H2O co-adsorption → N2 flushing and CO2&H2O co-adsorption → steam purge. Slight differences in XRD patterns could be observed for the sorbents processed with these procedures. The stable sorption capacities over long cycles of adsorption/desorption are due to the fast desorption kinetics. From a micro-view, the CO2 needs to be removed from a special adsorption site in order to maintain stable sorption capacities. These results can significantly help understand the stability of the potassium-promoted hydrotalcite-based adsorbent and the design of different sorption processes.

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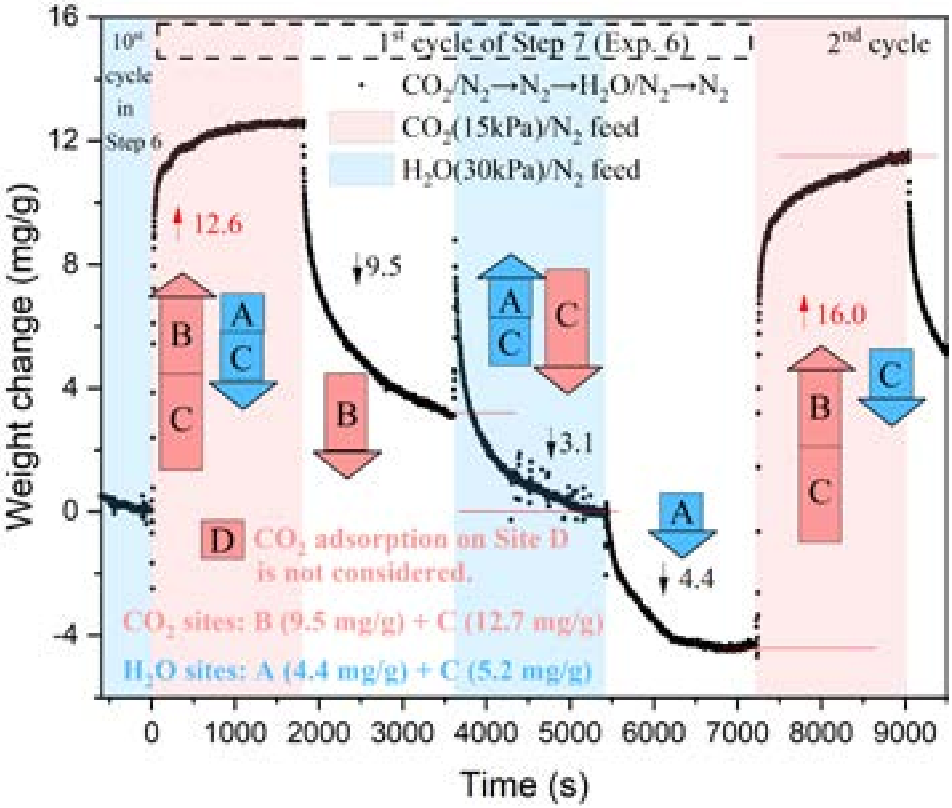

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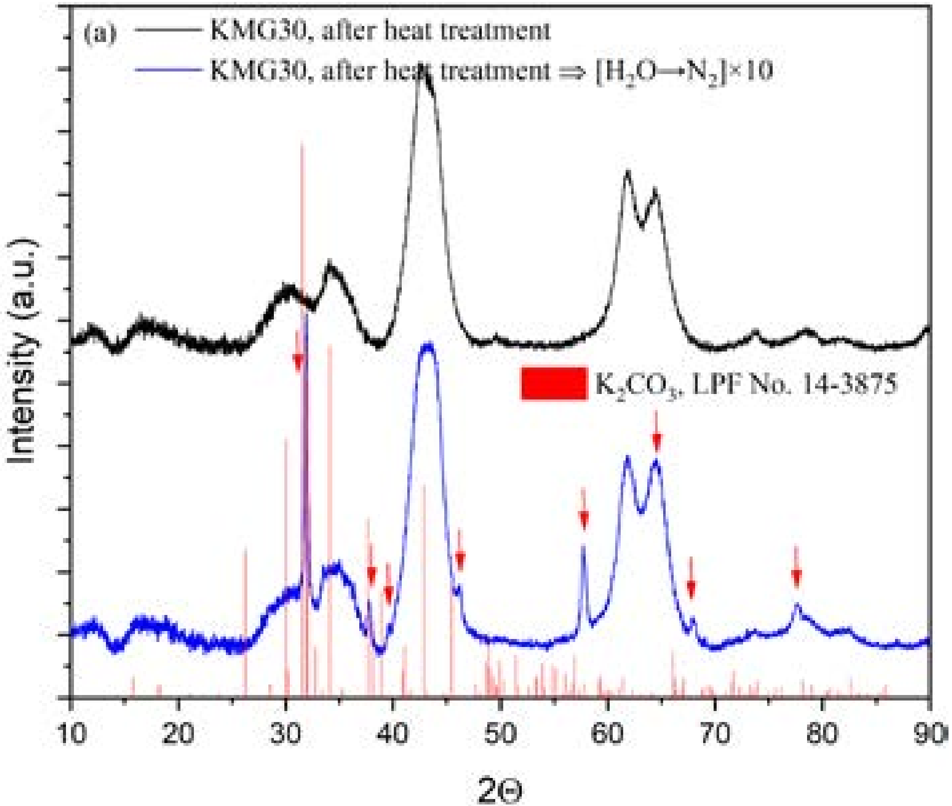

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Author: Eline van Daatselaar (UTwente)

Other Authors: A.G.J. van der Ham, University of Twente; S.R.A. Kersten, University of Twente; M.P. Ruiz, University of Twente

Title: **[L34] Chemical recycling of plastic waste: from polyolefins to short alkanes via hydrogenolysis**

Abstract: The worldwide production of fossil-based plastics has significantly increased in the last years, up to 352.3 MTons in 2022 [1]. This increasing demand urges the development of competitive technologies for mechanical and chemical recycling of plastic waste. In this work, we focus on the hydrogenolysis of polyolefins as a potential alternative for chemical recycling of plastic waste to valuable products (e.g., naphtha fraction). Recent literature has shown that hydrogenolysis of polyolefins (PE, PP) over e.g., Ru/C catalyst at 200-300°C and 20-60 bar H2 can lead to liquid products, but it requires long reaction times (16 to 96 hours) [2]–[6]. In this study, by running experiments in a 40 mL stirred batch autoclave with the same catalyst at several feed-to-catalyst ratios, we show that the reaction time can be significantly shortened, resulting in full conversion of LDPE, HDPE and PP at 250-280°C and 40-60 bar H2, in time frames of 40 minutes to 4 hours. Products were analysed by both gas chromatography (GC) and gel permeation chromatography (GPC). Products for polyethylene are mainly gaseous and short alkanes, whereas polypropylene gives higher molecular weight products. For example, hydrogenolysis of LDPE (MW 4 kDa, 250°C, 40 min, 40 bar of initial hydrogen pressure, feed-to-catalyst ratio 9.3), gives a gas (C1-C4) yield of 17.6 wt.% and a liquid (C5-C33) yield of 30.5 wt.%, see figure. In parallel, a model describing the (random) scission of the polyolefins during hydrogenolysis is developed, making eventually the prediction of the product distribution possible. The combination of the experimental results and the ability to predict the product distribution based on process conditions show that implementing smart reactor and process design could increase the feasibility of hydrogenolysis to retrieve useful carbon compounds from plastic waste. References:

[1] Plastics Europe, 2021.
[2] J. E. Rorrer et al., JACS Au, vol. 1, no. 1, pp. 8–12, Jan. 2021, doi: 10.1021/jacsau.0c00041.
[3] J. E. Rorrer et al., ACS Sustain. Chem. Eng., vol. 9, no. 35, pp. 11661–11666, Sep. 2021, doi: 10.1021/acssuschemeng.1c03786.
[4] P. A. Kots et al., ACS Catal., vol. 11, no. 13, pp. 8104–8115, 2021, doi: 10.1021/acscatal.1c00874.
[5] Y. Nakaji et al., Appl. Catal. B Environ., vol. 285, no. September 2020, p. 119805, 2021, doi: 10.1016/j.apcatb.2020.119805.
[6] G. Celik et al., ACS Cent. Sci., vol. 5, no. 11, pp. 1795–1803, Nov. 2019, doi: 10.1021/acscentsci.9b00722.”

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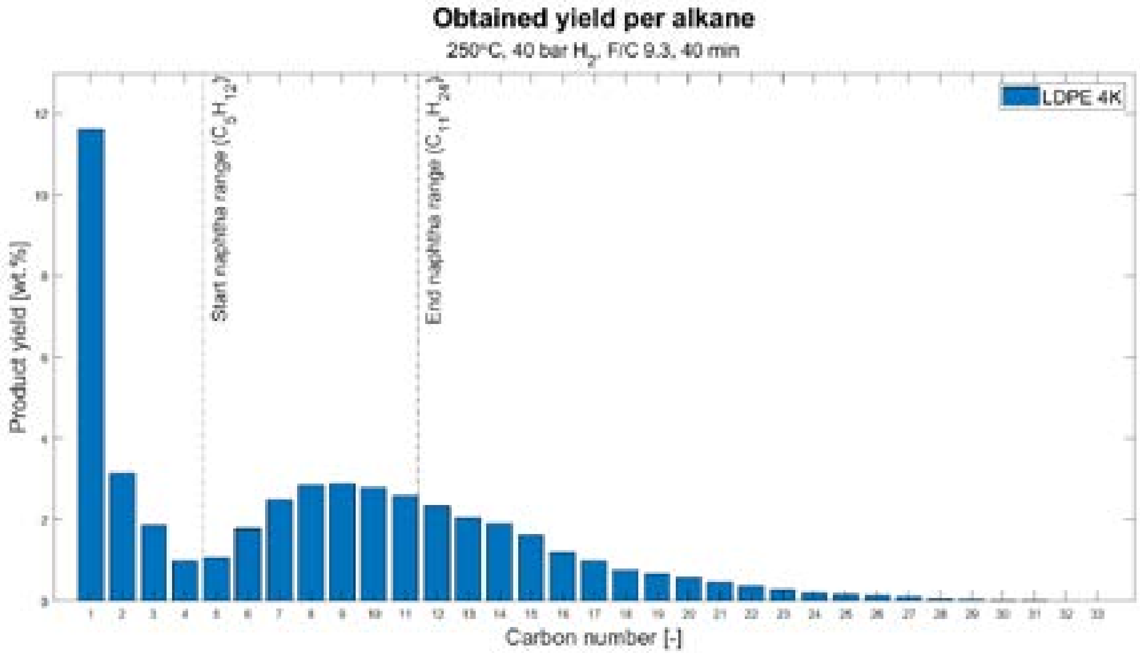
Obtained yield per alkane
250°C, 40 bar H_2, F/C 9.3, 40 min
LDPE 4K
Start naphtha range (C_5H_{12})
End naphtha range ($C_{11}H_{24}$)
Product yield [wt.%]
0
2
4
6
8
10
12
Carbon number [-]
1
2
3
4
5
6
7
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Author: Elchin Jafariyeh Yazdi (RUG)

Other Authors: Jun Yue, University or Groningen; Gert-Jan Euverink, University or Groningen

Title: **[L35] Cellulase enzyme recovery from cellulosic hydrolysate**

Abstract: The depletion of fossil fuels and increasing awareness of global warming has engaged governments, companies and the scientific community to search for environmentally benign chemicals derived from renewable resources. Cellulose is the most abundant biopolymer and therefore an excellent source for the production of these chemicals. The utilization of cellulose derived from lignocellulosic feedstock is currently widely investigated in bioethanol production (1).Acid hydrolysis and biological saccharification are two approaches of biomass conversion to fermentable sugars. Enzymatic hydrolysis of biomass using cellulase enzymes to reduced sugars is a more sustainable method. It can be performed under mild temperatures resulting in higher selectivity to sugars that can be versatile platform for biobased chemicals (2). However, the high cost of enzymes continues to be a key impediment for the commercialization of the biomass conversion process. It is estimated that enzymes alone account for 50% of hydrolysis costs (3). Recycling enzymes is one way to reduce the overall enzyme consumption and increase enzymatic performance. In this way, the recovered enzymes in the hydrolysate can be reused to hydrolyze a fresh substrate. In this work, we have investigated the use of membrane filtration for the recovery of commercial cellulase enzymes. The membrane filtration technique can be a feasible method for recovering cellulase enzymes and simultaneously removing the end product produced from hydrolysis. Microcrystalline cellulose (Avicel) has been used as a representative of pure cellulose for the hydrolysis experiments in this work. Upon the completion of hydrolysis, all the unconverted solids were centrifuged out. Next, we used the Vivaspin centrifugal tubes for the purpose of filtration. We further investigated the activity of these recycled enzymes in a fresh reaction run, at both high and low solid and enzyme loadings.Our results show that liquid cellulase recycling is technologically feasible using membrane filtration. However, the initial rate and final conversion of hydrolysis were altered by using the recycled enzymes. After the first cycle of filtration, the recycled enzyme showed comparable performance to its initial condition. However, the performance of recycled enzyme after second cycle of filtration is declined. This decline in activity is drastic with low enzyme loadings, especially when the cellulose loading was relatively high. While in the case of high enzyme loadings, at least two successful recycling’s of cellulase are possible. The protein activity loss is greater for the third cycle at high enzyme loadings. Further studies to elaborate on the detailed behavior of cellulase enzymes in this process is under investigation.

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Other Authors: S.R.A. Kersten, University of Twente; M.P. Ruiz, University of Twente

Title:

[L36] Exploring the Intrinsic Kinetics of Polyolefins Pyrolysis in a Screen Heater Reactor

Abstract:

The kinetic of polyolefins pyrolysis has been the subject of numerous studies but the intrinsic value remains relatively unknown. Our research aimed to investigate the intrinsic kinetic of polyolefins pyrolysis by fitting experimental data to a lumped kinetic model. Different types of polyolefins (HDPE and LDPE) were pyrolyzed using a screen heater reactor, which offers very fast heating and quenching rates, and minimizes the impact of secondary reactions, mass transfer, and heat transfer on the reactions. This allowed us to obtain a more accurate determination of intrinsic kinetics. Additionally, the effect of initial molecular weight and pressure was also investigated. The experimental data were used to establish a first-order kinetic model that predicts the yield distribution of condensable (liquid oil and wax) and gas products. The overall kinetic constants obtained were approximately 0.5 s^-1 for HDPE and 1.3 s^-1 for LDPE, which are significantly higher than the reported apparent kinetic values in the literature. This study provides new insights into the kinetic behavior of polyolefins pyrolysis and the impact of feedstock properties and process conditions on the reaction. The results of this study have the potential for industrial applications, such as the design of pyrolysis reactors with improved heat transfer to achieve a more efficient process.

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Author: Shahab Zamani Gharaghooshi (UTwente)

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Title: **[L37] Chemical Recycling of Polyurethanes: Conversion of Carbamates**

Abstract: The increasing demand for polyurethanes has urged the development of technologies to process polyurethane waste. Being a thermoset, polyurethane is not amendable to mechanical recycling strategies, such as melting. Therefore, recycling is limited to downcycling through crushing and shredding to produce filler materials. Numerous studies have explored the chemical recycling of polyurethanes toward producing their monomers, i.e., polyols and isocyanates [1–3]. Split-phase glycolysis [2] and alcoholysis have shown promising results in the recovery of polyols and a complex mixture of aromatic species that can eventually be converted to isocyanates via phosgenation. i.e. through reaction with highly toxic phosgene. As an alternative to that route, the recovery of polyols has been investigated relatively well in literature; however, there are scarce studies focused on the recovery of the isocyanates. This work focuses on investigating and evaluating alternative routes for recycling polyurethanes to polyols and isocyanates without using phosgene as a reactant. To do so, the recycling routes are targeting the conversion of the aromatic components to carbamates, which have been reported to be converted to isocyanate under well-designed conditions. To this end, we are studying the decomposition of a model carbamate compound (Methyl N-phenyl carbamate) in thermal and catalytic cleavage processes under different operating conditions (180°C- 400°C), targeting the production of isocyanates.

[1] Y. Deng, R. Dewil, L. Appels, R. Ansart, J. Baeyens, Q. Kang, Reviewing the thermo-chemical recycling of waste polyurethane foam, J Environ Manage. 278 (2021) 111527. https://doi.org/10.1016/j.jenvman.2020.111527.

[2] J. Datta, M. Włoch, Recycling of Polyurethanes, 2017. https://doi.org/10.1016/B978-0-12-804039-3.00014-2.

[3] D. Simón, A.M.M. Borreguero, A. de Lucas, J.F.F. Rodríguez, Recycling of polyurethanes from laboratory to industry, a journey towards the sustainability, Waste Management. 76 (2018) 147–171. https://doi.org/10.1016/j.wasman.2018.03.041.”

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Author: Vikram Korede (TU Delft)
Other Authors:

Title: **[L38] Growth dynamics of aspirin crystals in microfluidic antisolvent crystallization**

Abstract: Controlling crystal size is a significant challenge for industrial crystallization with direct implications on product quality of essential crystalline materials ranging from pharmaceuticals to explosives. We explored controlling crystal size in antisolvent crystallization by dictating coupled mass and momentum transfer in microfluidic flows. In these experiments, a poor solution, saturated with aspirin, replaces a good solution in the microfluidic channel, which leads to a supersaturation pulse that moves through the channel and induces the growth of aspirin seeds. The hypothesized supersaturation pulse could be visualized by measuring the linear growth rate during the experiment. The experimental results show that the linear growth rate scales with Peclet number, in line with a theoretical scaling argument considering convection-diffusion balance and boundary layer behavior around a crystal. At large Peclet, a deviation from predicted scaling is observed which we attribute to changing dispersion behavior. Combining experiments and theory, we propose a quantitative tool to control crystal size in antisolvent crystallization.

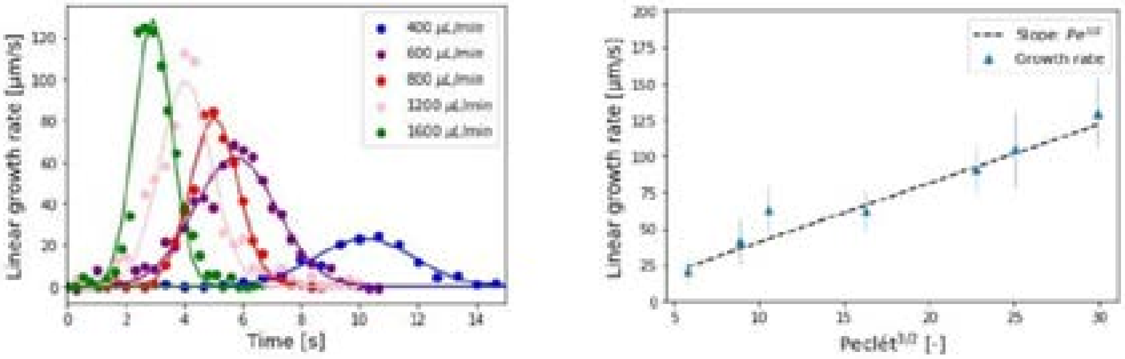

Figure 2: (A) The development of the linear growth rate over time for five different flow rates (400, 600, 800, 1200 and 1600 µL/min), here the linear growth rate resembles the expected form of a supersaturation pulse (B) Relationship between maximum linear growth rate and Pe in experiments at high supersaturation for flow rates 300, 400, 450, 600, 750, 800 and 900 µL/min. The trend resembles the relation dR/dt ~ $Pe^{3/2}$ which is expected to be a result of both boundary layer behaviour and a difference in mixing time

000002-Q-antisolvent-crystallization-figures.jpg

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Author: Federico Perondi (RUG)

Other Authors: Francesco Picchioni, University Of Groningen; Jun Yue, University Of Groningen; Michael Polhius, AVEBE innovation center

Title: **[L39] Supercritical Drying Of Starch**

Abstract: Drying is undoubtedly one of the oldest methods that have been applied for centuries in the preservation of primary agricultural commodities such as fruits and vegetables. Reducing free water content is a crucial factor in a product's shelf life that inhibits both the growth of microorganisms and biochemical enzymatic reactions. Several food drying techniques are in use in the last decades, but air drying (generally above 120 °C) stays as the most commonly used drying operation in the food industry. Recently, the use of CO2 at supercritical state (73 bar, 32 °C) has been investigated as an alternative drying process. Supercritical CO2 (ScCO2) drying induces minor capillary stresses with respect to conventional methods because the vapor-liquid interface is avoided, allowing the maintenance of the original structure. This also allows to lower the operating temperature compared with the oven drying, and thus theoretically less energy for the drying process (especially when CO2 is recycled). So far, the use of ScCO2 for drying purpose is already known in the literature, but a limited number of examples are reported1,2. In collaboration with AVEBE, the possibility of drying potato starch with ScCO2 is being studied in this project. The drying process has been studied in both batch and continuous flow reactors in order to study the influence of relevant operating parameters and thermodynamics. During these experiments, it was possible to obtain data for the solubility of water in ScCO2, as well as the effects of the main parameters (e.g., temperature, pressure and flow rate) on the drying process. Furthermore, the influence of CO2 drying on the obtained starch morphology/structure was also investigated via dedicated characterization such as XRD, SEM and RVA.

Literature

1. Brown ZK, Fryer PJ, Norton IT, Bakalis S, Bridson RH. Drying of foods using supercritical carbon dioxide - Investigations with carrot. Innov Food Sci Emerg Technol. 2008;9(3):280-289. doi:10.1016/j.ifset.2007.07.003
2. Zambon A, Tomic N, Djekic I, Hofland G, Rajkovic A, Spilimbergo S. Supercritical CO2 Drying of Red Bell Pepper. Food Bioprocess Technol. 2020;13(5):753-763. doi:10.1007/s11947-020-02432-x

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Author: Menno Houben (TU/e)

Other Authors: Thijs Jansman, TU/e; Zandrie Borneman, TU/e; Kitty Nijmeijer, TU/e

Title: **[L40] Layer-by-layer modified electrospun bipolar membranes for enhanced water dissociation**

Abstract: Lactic acid, an important material in the food industry, is often produced by fermentation. However, during fermentation mostly lactate salts are formed instead of lactic acid. Electrodialysis with bipolar membranes has the potential to convert lactate salts into lactic acid without the introduction of other chemical reagents by utilizing the water dissociation at the interface of the anion and cation-exchange layer of the bipolar membrane (BPM). Tailoring this interface of the BPM is thus essential to promote high water dissociation rates. Electrospinning allows larger control over the BPM interface thickness, morphology and composition compared to conventional casting techniques. In this work electrospinning is used to tailor the interface of the BPM to increase the compatibility and the surface area between the two ion-exchange layers resulting in increased water dissociation rates. To allow water dissociation to occur via both acid and base catalyzed mechanisms, polymeric water dissociation catalysts with a range of pKa’s are introduced at the electrospun interface by a layer-by-layer (LbL) modification approach with a polyethyleneimine (PEI)/polyacrylic acid (PAA) polyelectrolyte couple. SPEEK (cation-exchange layer, CEL) and FAA-3 (anion-exchange layer, AEL) nanofiber mats were prepared by wire-electrospinning. From these nanofiber mats dense BPMs were fabricated by stacking SPEEK and FAA-3 mats on top of each other and subsequent hot-pressing, resulting in an entangled small interface with a high active surface area (Figure 1). The polymeric water dissociation catalysts were introduced at the interface of the BPM by coating 1 electrospun SPEEK layer using the LbL method with PEI-PAA (Figure 2). The LbL assembly was characterized using optical reflectometry and showed an increase in layer mass per adsorption step. Furthermore, the adsorbed amount per layer was strongly dependent on the coating conditions (ionic strength and pH). This shows that the amount of catalytic sites at the interface of the BPM can be controlled by the amount of coating layers and the coating conditions. The electrospun BPM showed an improved performance compared to the conventional laminated BPMs due to this well entangled small interface between the anion and cation-exchange layer. Furthermore, the LbL coating significantly reduces the potential required for water dissociation. This potential drops from 5.2V for the pristine electrospun BPM to 2.4V for the LbL-coated electrospun BPM at 10mA/cm2, thus substantially enhancing the performance of these membranes. This work demonstrates the potential of bipolar membranes with enhanced performance due to the incorporation of catalytic sites with different pKa’s compared to conventional laminated bipolar membranes.

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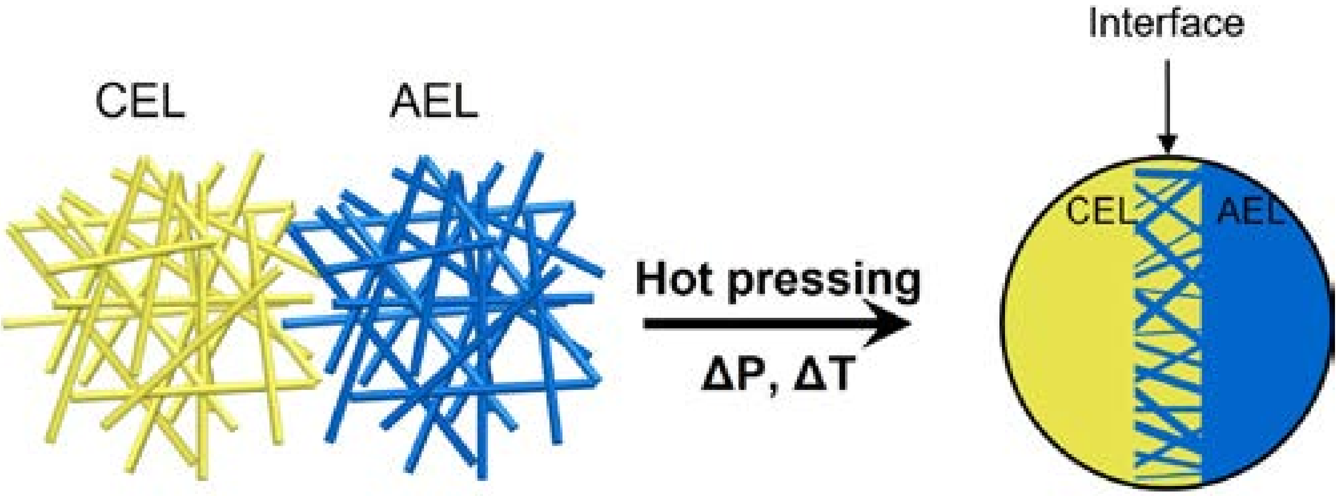
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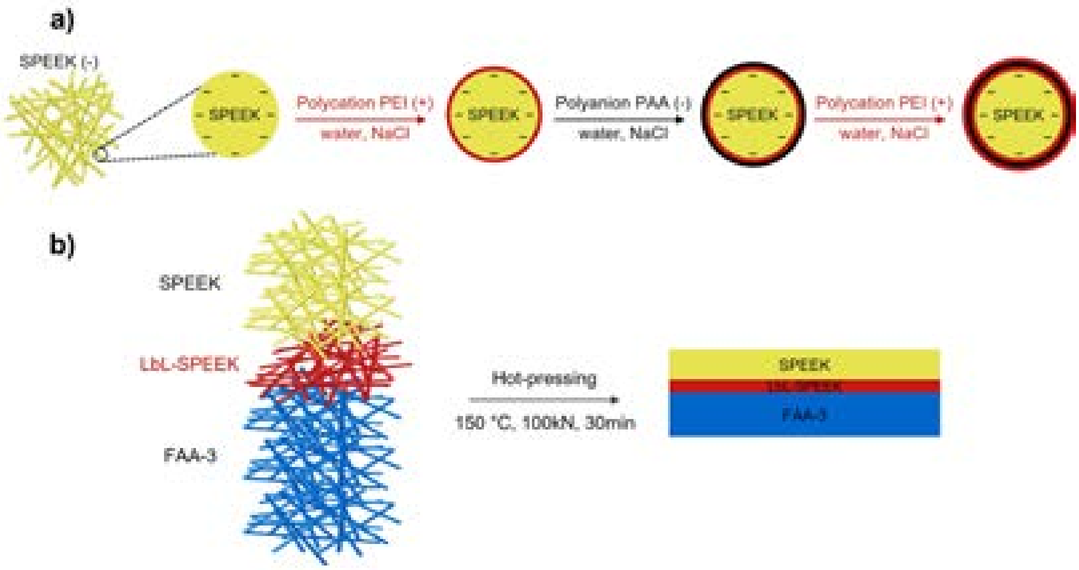
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Polycation PEI (+)
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SPEEK
b)
SPEEK
LbL-SPEEK
FAA-3
Hot-pressing
150 °C, 100kN, 30min
SPEEK
LbL-SPEEK
FAA-3

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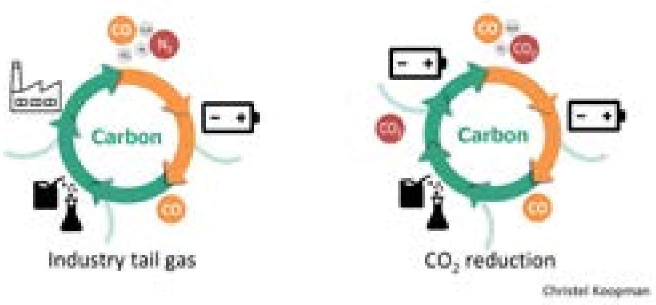
Other Authors: Jelco Albertsma, TU Delft; Monique van der Veen, TU Delft; David Vermaas, TU Delft

Title: **[L41] Electrochemically mediated carbon monoxide separation**

Abstract: Carbon monoxide is an essential feedstock for the production of higher value chemicals and fuels. At the same time, carbon monoxide is a by-product of some industrial processes as well as the product of electrochemical carbon dioxide reduction. Therefore, as part of the transition to a circular carbon economy, there is a need for cost- and energy-efficient separation of carbon monoxide. Conventional separation methods fail to efficiently separate carbon monoxide, resulting in flaring of carbon monoxide-containing tail gases. Especially the separation of carbon monoxide from nitrogen is challenging because of their similar physical properties, such as boiling point and size. Electrochemical separation could prove to be a suitable and efficient alternative due to direct supply of electrical energy to the active sites for separation as well as the potential to operate at ambient temperatures and generate high pressure product streams. In this project, we aim to design an electrochemical process to separate carbon monoxide from gas mixtures. Taking inspiration from nature, we will use the binding affinity of carbon monoxide to transition metals (such as iron), which changes with oxidation state. As a result, we can use electrochemistry to switch between a high affinity and low affinity state of the sorbent material. This can be implemented in an electro-swing adsorption process (schematic) or an electrochemically mediated absorption process. That is, we will use redox-active transition metal complexes to separate carbon monoxide from gas mixtures.



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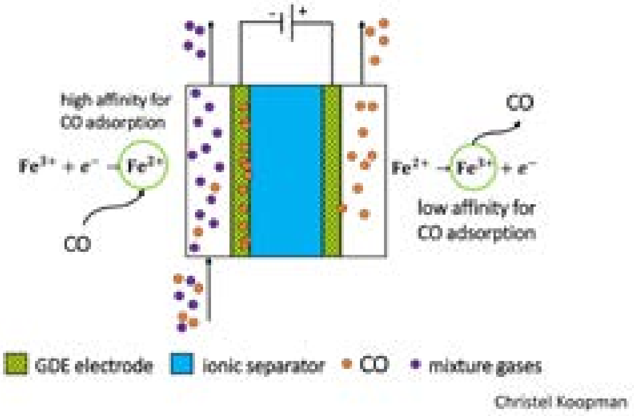

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Other Authors: D. A. Pacheco Tanaka, TECNALIA; M. A. Llosa Tanco, TECNALIA, B; F. Gallucci, TU/e

Title: **[L42] Carbon Molecular Sieve Membranes for separation of Helium from Natural Gas**

Abstract:

In recent years the demand for helium has been increased drastically. Helium is used in applications such as ultra-low temperature cooling [1], and for characterization techniques [2]. Unfortunately, despite the abundance of this element in the universe, currently there is only one commercial method to extract this crucial element. Helium exists in mixture of other gases such as methane, nitrogen, carbon dioxide and etc. in the natural gas reservoirs. In extraction of natural gas, helium is also co-extracted and then purified in a multi-stage process to reach the acceptable level of purity to be used in industries [3]. Due to the extremely high power consumption and existence of multiple steps of purification, currently the price of helium is significantly increasing and due to low existing concentration of helium in natural reservoirs, the price is expected to increase in coming years [4]. Membrane separation technology is considered one of the novel methods in helium separation and purification. The required high prem-selectivity in the membranes limits the candidates for this application from polymeric membranes. Moreover, the co-existence of H2S and CO2 in the gas mixture, results in reduction of the performance of polymeric membranes in long term use [5]. Carbon molecular sieve membranes (CMSMs) are fabricated via pyrolysis of a thermosetting polymer under inert atmosphere. The resulted porous material could be used as a membrane to separate molecules with different kinetic diameter from each other. CMSMs are fabricated with resorcinol-formaldehyde precursor for separation of helium from natural gas mixture. Alpha alumina tubular supports were used for dip-coating of polymeric solution and then after polymerization-drying step, were carbonized in temperatures of 700-850°C. The effect of carbonization temperature on the performance of the membranes were evaluated based on perm-selectivity tests and pore size distribution characterization. CMMS with extremely high perm-selectivities at temperatures of 5, 10, 15 and 20°C were fabricated and tested up to 40 bar pressures. The performance of CMSMs, passed Robeson’s upper bound limit of polymeric membranes. Figure 1, effect of carbonization temperature on pore size distribution and He/CH4 ideal selectivity in CMSMs.
The increase in carbonization temperature, enhances He/CH4 ideal selectivities in CMSMs which is in accordance to PSD measurements with the smallest average pore size in CMSM carbonized at 850°C.

References

1. Baxi CB, Wong CP. Review of helium cooling for fusion reactor applications. Fusion Engineering and Design. 2000 Nov 1;51:319-24.
2. Wirtz T, De Castro O, Audinot JN, Philipp P. Imaging and analytics on the helium ion microscope. Annual Review of Analytical Chemistry. 2019 Jun 12;12:523-43.
3. Dai Z, Deng J, He X, Scholes CA, Jiang X, Wang B, Guo H, Ma Y, Deng L. Helium separation using membrane technology: R”

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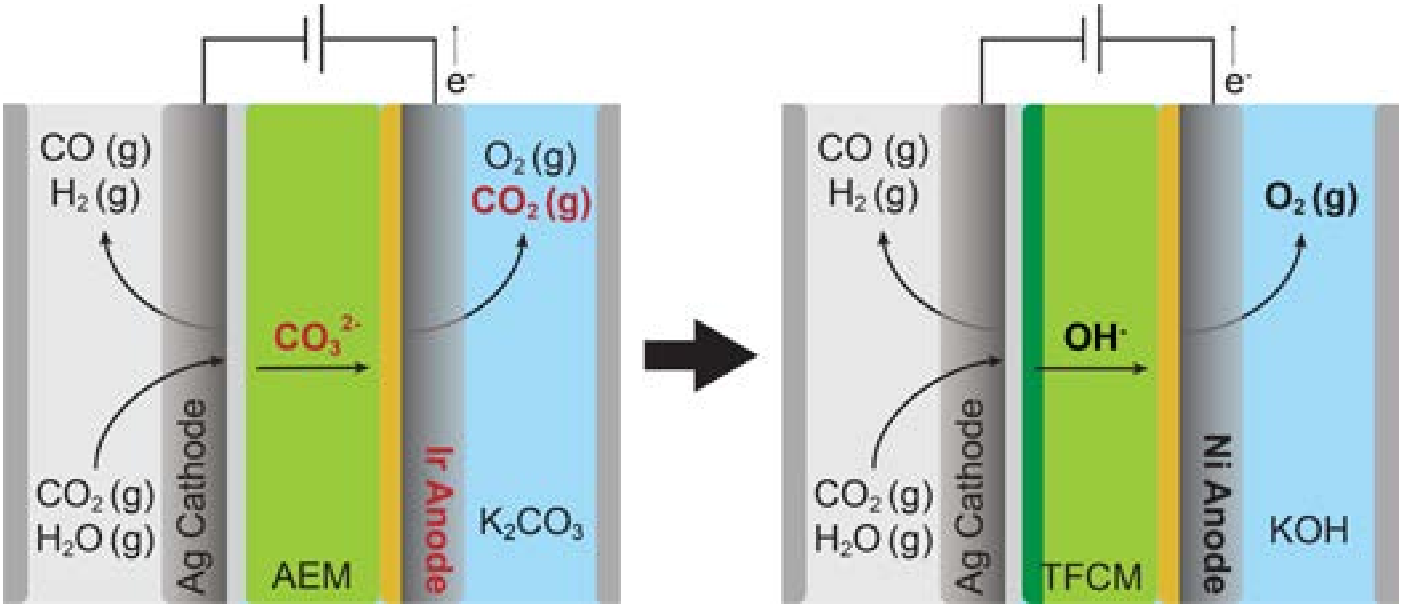
Author: Kostadin Veselinov Petrov (TU Delft)

Other Authors: Teise Stellema, TU Delft; David A. Vermaas, TU Delft

Title: **[L43] OH- selective thin film composite membranes can prevent CO2 loss in CO2 electrolysis**

Abstract: The rise of wind and solar renewable energies has stimulated development of electrochemical conversion processes, such as water and CO2 electrolysis, and fuel cells. Large-scale CO2 electrolysis could allow the sustainable production of fuels and chemicals while offering means to store renewable energies. Currently, the main challenge of this technology is the carbonate cross over. At the cathode, the CO2 reduction reaction generates OH- which in turn reacts with CO2 producing carbonate (CO32-) and bicarbonate (HCO3-). This (bi)carbonate crosses over to the anolyte via the anion-exchange membrane which acts as conductive separator, and turns back to CO2, compromising the overall conversion and efficiency of the process. To solve this challenge, we've synthesized an OH- selective anion-exchange membrane which can reject (bi)carbonate. This was achieved by modifying a commercial IEM with a thin polyamide selective film. This layer, typically used in reverse osmosis membranes for water desalination, is synthesized on the surface of the membrane through an interfacial polymerization reaction. Our results show that these thin film composite membranes can successfully reject over 85% of carbonate ions, with only a small compromise of their hydroxide conductivity. In this presentation we will highlight the challenges of integrating such a membrane in a CO2 electrolyzer and how a CO2 electrolyzer with no CO2 loss can be achieved.



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Author: Senan F. Amireh (TU/e)

Other Authors: Antoni Forner-Cuenca, TU/e

Title: **[L44] Engineering gas diffusion electrode microstructures for the electrochemical reduction of CO2 to ethylene**

Abstract: The electrochemical reduction of CO2 is a promising technology for the production of clean and sustainable chemicals and fuels through the utilization of captured CO2. However, there are several challenges such as limited operational times and low current densities, which need to be overcome for commercialization [1]. The implementation of gas diffusion electrodes (GDEs) is a key advancement which enabled higher current densities since the porous structure facilitates efficient gas diffusion to the catalytic surface. However, the current state-of-the art GDE materials have been repurposed from low temperature fuel cells and, while functional, these GDEs have not been tailored for the specific requirements of emerging CO2 electrolysis cells. The GDE microstructure and surface properties are unsuited to sustain the growing requirements of CO2 electrolysis flow reactors. Consequently, the GDEs suffer from flooding through different mechanisms such as electrowetting [2], capillarity [3], salt precipitation [3], and uneven pressure distribution [4]. Therefore, there is a need for tailored GDEs with controlled microstructure and hydrophobicity. In this project, we aim to understand the role of the GDE microstructure on the performance of CO2 electrolysis to produce ethylene. Instead of leveraging commercial, carbon fiber-based substrates, we will manufacture our own GDEs using a scalable technique. By controlling synthetic parameters, we aim to engineer the pore size distribution, porosity and wetting properties. Furthermore, we will correlate synthetic parameters with the resulting properties (e.g. microstructure, transport) and flow cell performance. We hypothesize that mass transport rates and flooding resistance can be improved by tuning the pore size distribution and surface energy of the surface, and that this could enable longer operational times and higher current densities. In this presentation, I will give an overview of this research and will discuss my recent progress in the development of tailored diffusion electrodes.

References

1. C. Chen, J. F. Khosrowabadi Kotyk, and S. W. Sheehan, Chem, 4, 2571–2586 (2018).
2. K. Yang, R. Kas, W. A. Smith, and T. Burdyny, ACS Energy Lett, 6, 33–40 (2021).
3. M. E. Leonard, L. E. Clarke, A. Forner-Cuenca, S. M. Brown, and F. R. Brushett, ChemSusChem, 13, 400–411 (2020).
4. L. M. Baumgartner, C. I. Koopman, A. Forner-Cuenca, and D. A. Vermaas, ACS Sustain Chem Eng, 10, 4683–4693 (2022).

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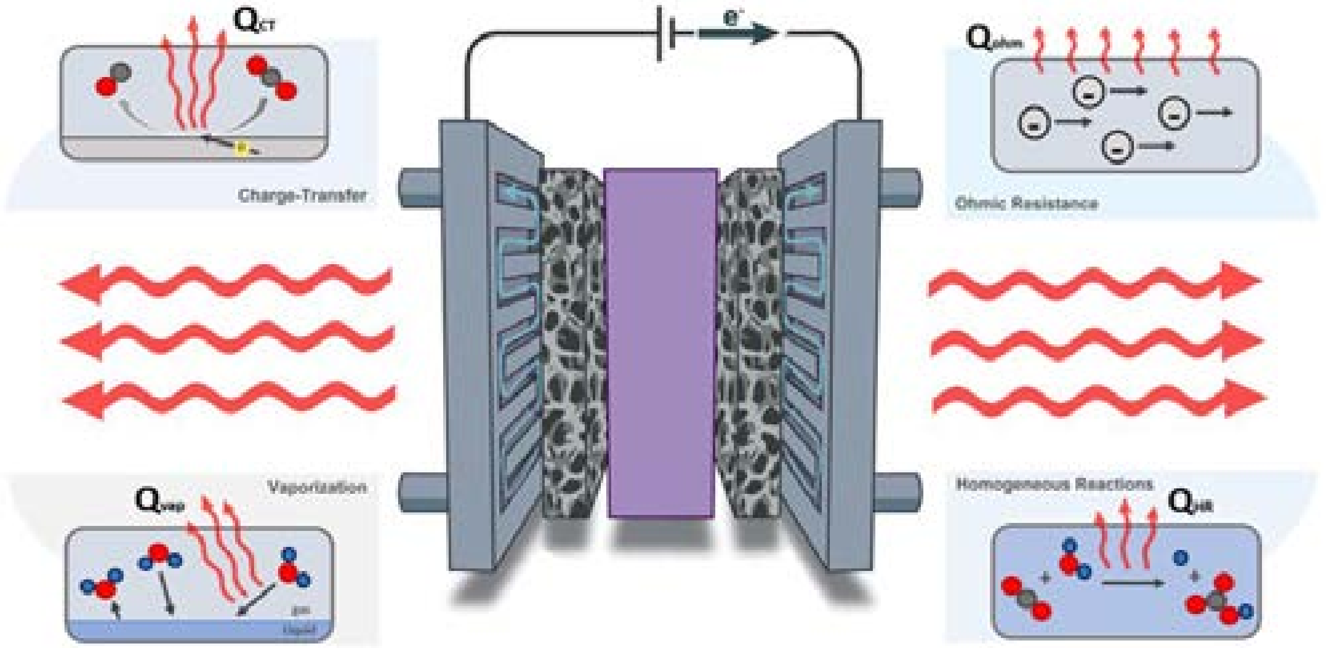
Author: Jan-Willem Hurkmans (TU Delft)

Other Authors: Jun Yue, University or Groningen; Gert-Jan Euverink, University or Groningen

Title: **[L45] Thermal implications in next-generation CO2 electrolyzers: a hot topic**

Abstract: Electrolysis offers a means to convert (renewable) electrical energy into chemical energy. Green hydrogen can be produced through the electrochemical reduction of water and carbon dioxide can be electrolyzed into valuable chemicals and fuels. However at industrially relevant scales and current densities, thermal effects are expected to introduce several challenges. Problems related to heat generation are expected to be amplified in systems for the electrochemical reduction of CO2, since they are often vapor-fed and exhibit relatively poor efficiencies. In order to accelerate the development of next-generation electrolysis technologies, it will be essential to understand and predict heat transfer in these systems. We do so by simulating scaled up electrolyzers through numerical methods. Results show that gas-fed CO2 electrolyzers can reach significant temperatures at industrially relevant current densities even for relatively small reactor dimensions. Additionally, our results show that non-isothermal effects can have a significant influence on the electrochemical performance of the systems dependent on the simulated reactor configuration.



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Author: Woutje ter Weel (TU/e)

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Title: **[L46] Anion exchange membranes for the electrochemical reduction of C)2**

Abstract: The electrochemical reduction of residual CO2 towards fuels and chemicals such as ethanol and ethylene is a promising route to lower our carbon footprint, especially when combined with renewable energy to drive the reactions. CO2 reduction is mainly performed in membrane-containing flow cells consisting of electrodes on opposite sides of an ion exchange membrane in an alkaline electrolyte solution (Figure 1). The ion exchange membrane should facilitate the transport of ions between the anode and cathode while serving as a chemical barrier between the two compartments. When operating in an alkaline environment, anion exchange membranes are preferred because their fixed positively charged ion exchange groups allow the transport of hydroxide ions from the cathode to the anode. Their main drawback lies in the cross-over of anionic reaction intermediates and poor chemical and mechanical stability at high pH. While extensive research has been performed on electrodes for CO2 reduction, it remains unclear how the membrane affects the CO2 reduction and which membrane-type is best performing. Therefore, we focused on studying six commercially available membranes which are characterized in terms of their chemical composition, ion exchange capacity (IEC), water uptake, permselectivity, and ionic conductivity. Fujifilm T1 and FAB-PK 130 show a trade-off between permselectivity and conductivity, often seen for AEMs. The high conductivity of Fujifilm T1 can be a result of its high water uptake, promoting ion transport. Neosepta AMX fg and Fujifilm T10 differ in their conductivity due to the higher water uptake of Fujifilm T10. The support of the FAA-3 PK 130 causes a lower water uptake compared to the unsupported FAA-3 50 but does not influence the IEC. FAB PK 130 and FAA-3 PK 130 have the same support but different cationic polymers explaining the lower IEC and water uptake for FAB PK 130 and thus the lower conductivity. A lower ionic conductivity will increase the resistance in the CO2 reduction cell, therefore, creating a less energy efficient system. Furthermore, diffusion experiments were performed to study the cross-over of CO2 reaction products (acetate, formate and ethanol) and anions from the electrolyte (carbonate, bicarbonate and hydroxide) over the different commercial membranes. FAB-PK-130 shows the lowest diffusion rate, attributed to its low water uptake and IEC. The high water uptake of Fujifilm T1 resulted in faster diffusion rates. This can result in a higher cross-over of CO2 reduction products over the membranes. As a consequence, the energy efficiency of the cell can decrease due to energy losses caused by the transport of reaction intermediates. Overall, the membrane is an important component of the CO2 reduction setup, which can influence the energy efficiency of the electrochemical cell and the product distribution in the electrolyte streams.

Acknowledgment: This work is part of the RELEASE research program

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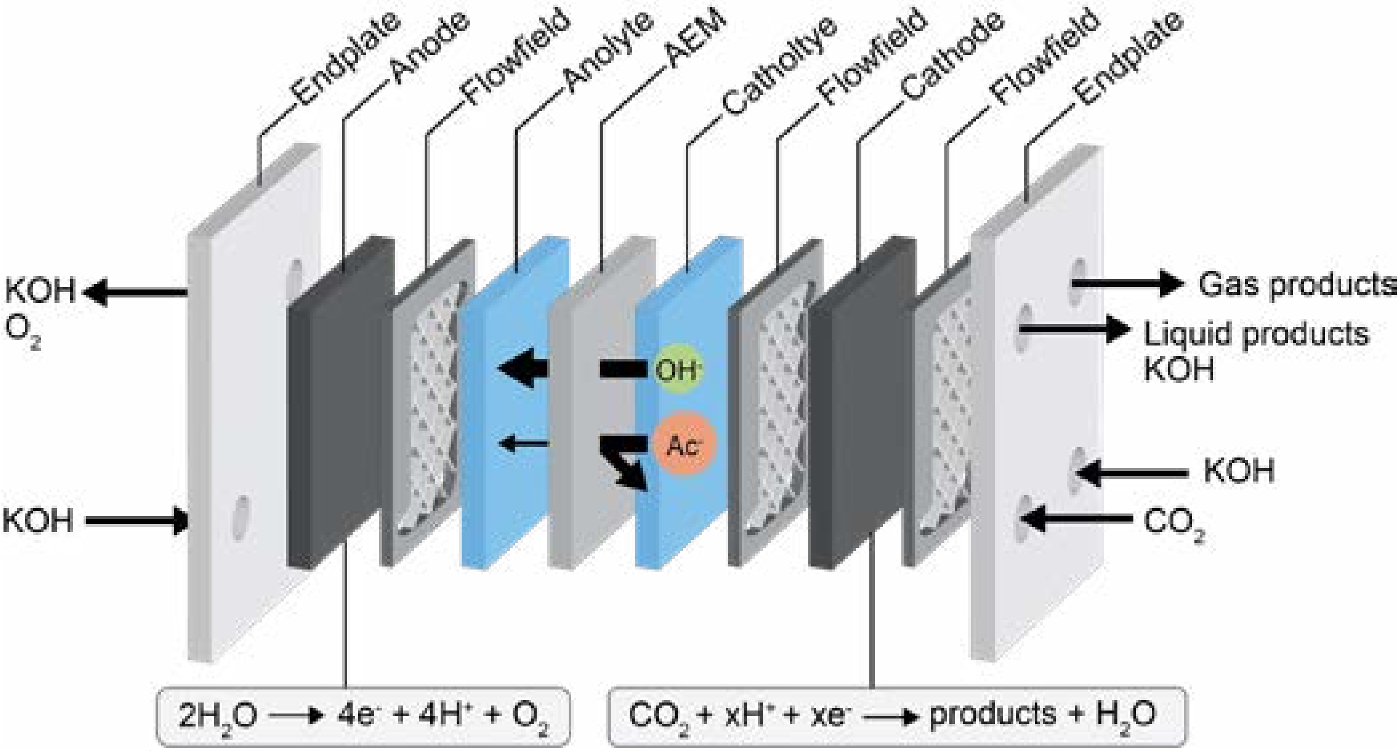

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Author: Michele Tedesco (TNO)

Other Authors: Gopalan Jayashankar, TNO; Javier Fatou Gómez, TNO; Simone Dussi, TNO

Title: **[L47] Modeling optimal operational strategies for alkaline electrolyser under dynamic power input conditions**

Abstract: Improving operational flexibility of electrolysers is one the major challenges to ensure large-scale implementation of green hydrogen production. In particular, when coupling electrolysers with intermittent energy sources, electrolysers need to be able to cope with dynamic power input conditions, while ensuring safe and stable operation. Identifying the optimal operating strategies for such dynamic situation is still a challenging task. In this work, we have adopted the model previously developed by de Groot et al. (Int. J. Hydrogen Energy 2022) to simulate the behavior of a 100 MW alkaline electrolyser coupled with different renewable energy sources (wind, solar, and their combination). Our model uses realistic energy profiles from wind and solar farms as power input, and predicts as output the optimal operating conditions for the electrolyser, in terms of pressure, temperature, minimum load and corresponding hydrogen production, curtailment and downtime. Our results show how – for a given electrolyser design – the nature of the energy source (i.e., wind, solar, or both) influences the total hydrogen production and downtime, as well as the optimal operational strategies. Such insights are useful from a system integration perspective, and emphasize how aspects such as electrolyser capacity and coupling with renewables should be taken into account to maximize the hydrogen production, and therefore improve the business case for hydrogen producers.

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Author: Jorrit Bleeker (TU Delft)

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Title: **[L48] Visualizing pH and mass transport in electrolyser with new FLIM probes**

Abstract: Information on pH and mass transport is essential in the optimization of emerging electrochemical technologies like water and CO2 electrolysis. The stability of earth abundant oxygen evolving electrodes, the selectivity of the reaction and the concentration CO2 are all strongly dependent on the local pH. Fluorescence Lifetime Imaging Microscopy (FLIM) is an imaging technique that can visualize the pH by adding a fluorescent probe to the solution. The technique was originally developed for biological systems and hence the commercially available probes are only pH sensitive at acidic and neutral conditions (pH 4-8). We have developed a new group of FLIM probes based on the 1-methyl-7-amino-quinolinium fluorophore. With relatively easy chemistry we can change R-group on the fluorophore which allows us to tune pH range in which the probe is sensitive. These quinolinium probes are sensitive to pH changes between 5 and 13, allowing for a whole new range of applications. This is especially interesting for visualizing the local pH in CO2 electrolysis, CO2 capture and alkaline water electrolysis, but the large pH range is useful for many other processes. As a proof of concept we have visualized the pH around a dissolving CO2 bubble in surrounding electrolyte, with a temporal resolution of 2-3 frames per second and a spatial resolution of 4 µm. We have also used our FLIM setup to investigate the pH boundary layer that forms in a water electrolyser. For every H2 molecule produced, two OH- ions are released and similarly at the oxygen evolving electrode OH- ions are consumed. Our initial results have shown that the mass transport is highest when a gas bubble is released from the electrode and that the boundary layer is not strongly affected by growth and coalescence of hydrogen and oxygen bubbles.

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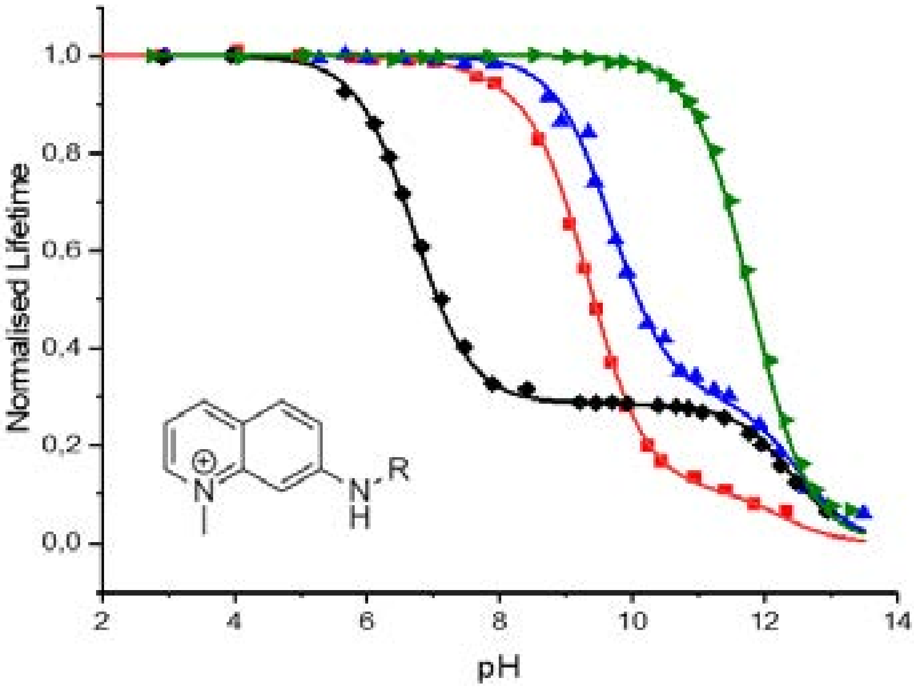

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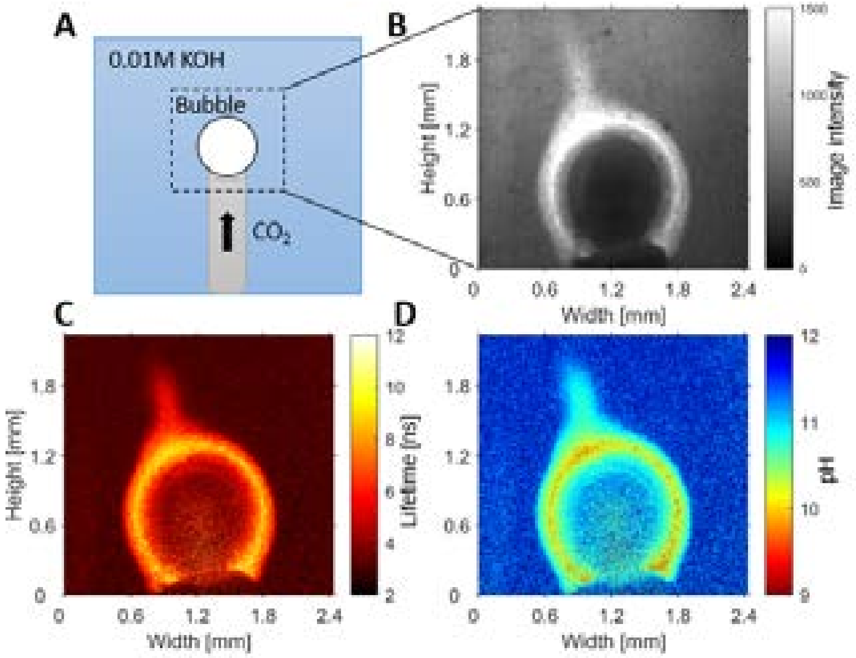

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Other Authors: J.A.M. (Hans) Kuipers, TU/e; K.A. (Kay) Buist, TU/e; M.W. (Maike) Baltussen, TU/e

Title: **[L49] 3D Air Bubble Shape Reconstruction from 2D Imagery using Neural Networks and Spherical Harmonics**

Abstract: Estimating the 3D shape of air bubbles in air-water bubbly flows from 2D imagery unlocks new possibilities to gain information on mass transfer in gas-liquid columns. Better understanding of the gas-liquid column's behavior results from extracting characteristics like the bubble area and volume from images. Using 2D images of single bubbles as input in a Convolutional Neural Network (CNN) the 3D shape is predicted. The prediction simplifies by representing the 3D bubble as spherical harmonic functions. Spherical harmonics decrease the number of output parameters by two orders of magnitude to approximately 250 coefficients. Figure 1 shows scaling single spherical harmonic orbitals by a coefficient and summing the results can accurately describe the 3D shape of an air bubble. Shape anomalies are caused by the Gibbs phenomenon or 'ringing' due to a limited number of spherical harmonic orbitals. Additional to forming the network labels during training, these simplified bubble representations helped synthesizing the training images in 3D software Blender. Recreating a pseudo 2D column in this program resulted in creating convincingly realistic 2D imagery. The accuracy of Blender's lighting properties was validated by experimental results. Both epipolar photography and photos from an epoxy bubble mall showed similarities to synthetic images from Blender. Currently the model performs decent by predicting a general 3D shape. The dimensions of the predicted shapes and test bubbles sample almost overlap. However, a shortcoming appears to be the absence of smoothness in the predicted surface. Moreover, difficulties arise when input images contain less spherical bubbles. These challenges might be overcome by image preprocessing to decrease the complexity of the task.

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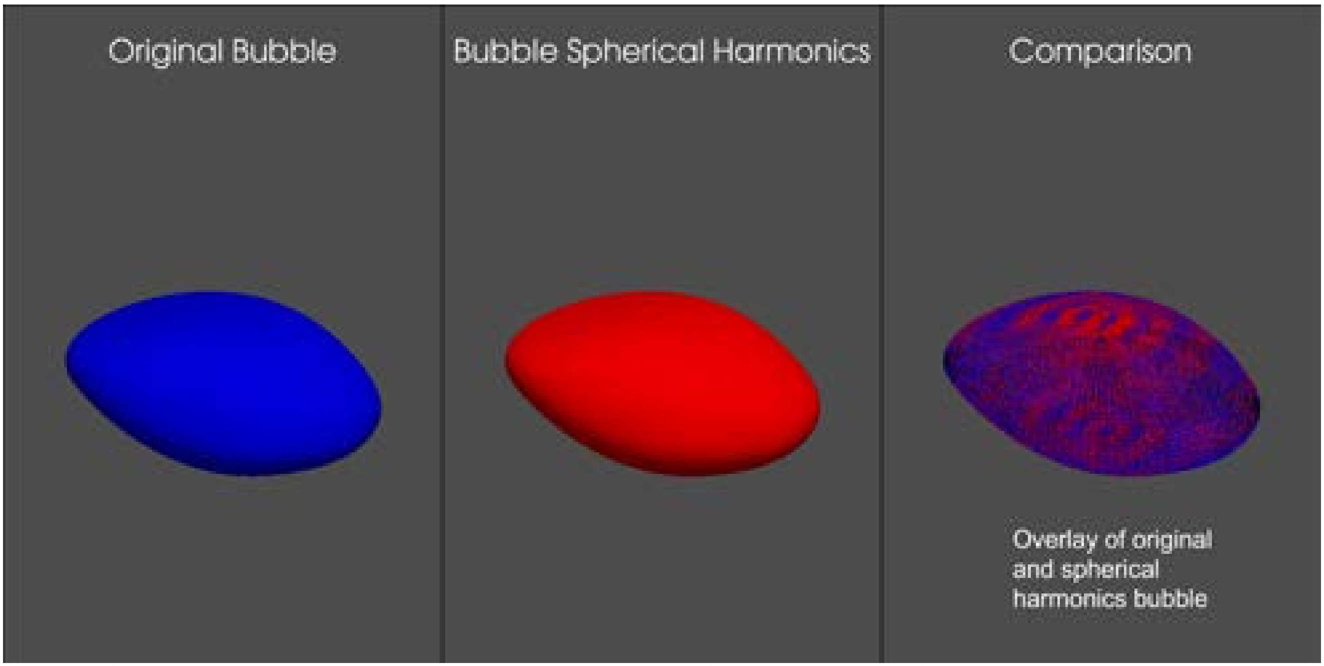

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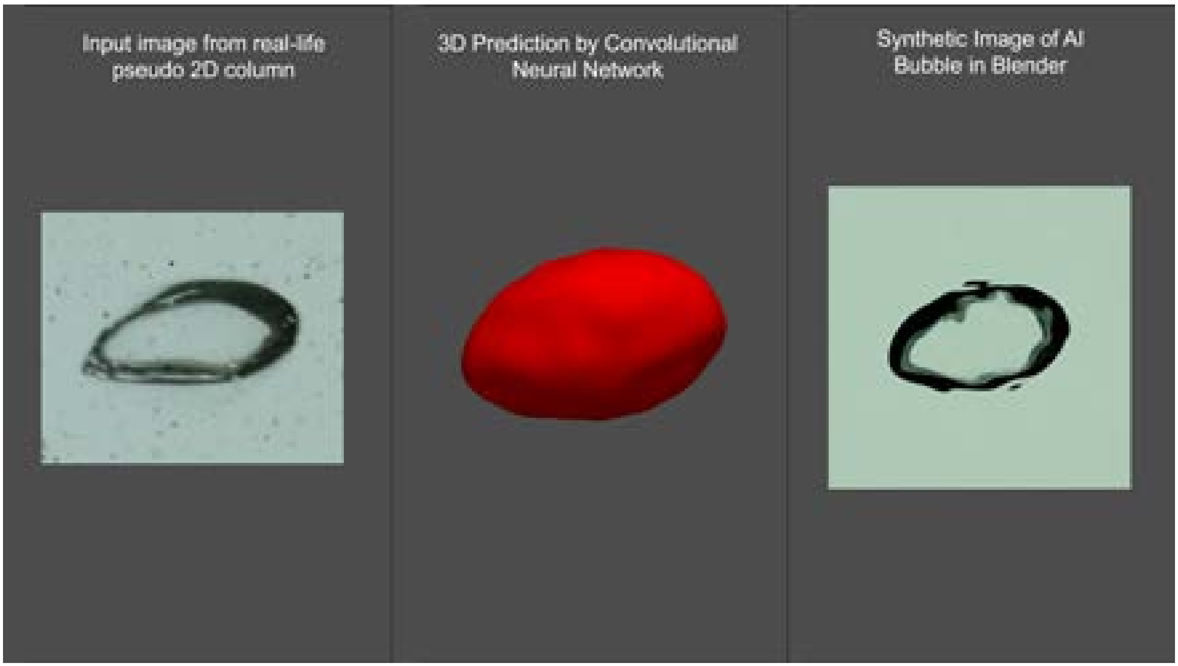

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Author: Valeria Garbin (TU Delft)

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Title: **[L50] Predicting the steady-state performance of Pickering emulsion reactors**

Abstract: Pickering emulsions, which are stabilized by nanoparticles instead of molecular surfactants, hold exciting potential as platforms for sustainable chemical conversion, promising higher conversion rates and selectivity, and easier catalyst recovery. The catalyst can be compartmentalized within the emulsion droplets, and the droplets can be packed into a column reactor with continuous flow of reactants in the continuous phase. Reaction products are immediately removed from the reaction site at the liquid-liquid interface, giving high conversion and selectivity. The overall performance of these novel reactors relies on the efficient mass transfer of reactants/products across the liquid-liquid interface and the interfacial layer of particles and the reaction kinetics. The bottleneck in predicting the optimal conditions is our limited understanding of effect of the layer of particles on mass transfer. To fill this gap, we developed a numerical model to describe pseudo-first order series reactions under steady state, where we investigated the effects of liquid properties, particle sizes and reaction kinetics, on the conversion and selectivity in a single Pickering droplet and the corresponding column reactor. By comparing with bare droplets, we link the microscopic properties of the particle-stabilized droplets and their dynamics, to the reaction performance. Such insights will ultimately contribute to control the performance of Pickering-emulsion reactors, paving the way towards optimized handling of complex, multiphase systems in continuous-flow Pickering emulsion.

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Title: **[L51] Study of the Hydrodynamics in a Trickle Bed Reactor using Particle-resolved Simulations**

Abstract: Trickle bed reactors are one of the most common reactors for processes involving gas-liquid-solid interactions. The performance of a trickle bed reactor is highly dependent on the hydrodynamics of the reactor which is governed by the particlescale transport phenomena. Therefore, thorough understanding of the hydrodynamics is essential for designing, optimizing and scale-up of trickle bed reactors. In this work, the knowledge on the hydrodynamics is extended using Direct Numerical Simulation (DNS), which combines a Volume of Fluid (VoF) method to represent the gas-liquid interaction and an Immersed Boundary Method (IBM) to represent the fluid-solid interactions. The gas-liquid-solid interactions are captured by applying contact angle boundary condition at the three-phase contact line. The study shows the effect of the liquid flow rate and the particle size on the liquid maldistribution and wetting efficiency in a randomly packed bed of particles.

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Other Authors: Ana Somoza Tornos, TUDelft; Giljam Bierman, TUDelft

Title: **[L52] Development of long-term Hydrogen storage technologies through green ammonia production in innovative Catalytic Membrane Reactor (CMR)**

Abstract:

Hydrogen produced from electrolysis offers great promises as energy carriers offering perspective for both short-and long-term energy storage. Ammonia is a perfect candidate as a new efficient way to produce long-term hydrogen storage since it offers a liquid storage of renewable electricity at ambient pressure and low boiloff conditions, while hydrogen can only be stored at scale in cavities and pipeline. The system design of the ammonia synthesis reactor poses a challenge due to the harsh reactor requirements for high inlet temperature to the reactor, which is necessary to achieve high reaction rate. Moreover, simultaneously, high operating pressure to achieve a high equilibrium conversion. In this project we want to develop a novel catalytic membrane reactor (CMR) that integrates the new NH3 selective membranes immersed in 3D printed Periodic Open Cellular Structures (POCS) where the new catalysts is coated/packed. Particularly, new carbon molecular sieve membranes (CMSM) are developed in order to selectively remove NH3 from the reaction mixture. Moreover, and a model reactor will be designed for in-situ reaction and separation, aiming to overcome the equilibrium limited reaction. A 1D reactor model have been developing based on previous kinetic study for Ru/C catalysts has been implemented in order to evaluate the performance of a membrane reactor as a function of the process parameters. The focus is on the identification of the required membrane properties, particularly permeability and selectivity, which can maximize NH3 yield and N2 conversion.

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Title: **[L53] Unraveling the impact of using alternative carbon feedstocks in existing petrochemical clusters**

Abstract: A future industrial system that is independent of fossil resources will require the use of alternative carbon sources (ACS), such as CO2 or biomass, to produce chemicals and materials. Industrial clusters are, however, complex systems with many and increasingly intertwined processes where interventions in any single process can affect other processes. There is, however, limited knowledge on the potential impact of deploying ACS processes in existing symbiotic industrial clusters. Without this knowledge, the use of ACS could unintentionally result in industrial systems that are more complex, less resource efficient, and produce more emissions. To address this gap, we are developing and testing a conceptual framework that combines ex-ante technology assessment and industrial symbiosis to understand cascading impacts. In this presentation, an overview of the methodology and intermediate results of the VICI project UNRAVELING (2019-2024) will be presented. In the first phase of the project, which has been completed, we developed a bottom-up model of a representative petrochemical cluster based on existing conditions in the Port of Rotterdam (PoR). The model includes 54 fossil base chemical processes (corresponding to 20 companies). Each individual process has been modeled using Aspen Plus, mimicking the characteristics of the existing plants in the PoR (e.g, in terms of type of products, technology routes, capacities, and utilities). This approach allows getting detailed energy and mass balances as well as equipment lists. Further, we identified and included in the model existing interactions between chemical processes in terms of product, energy (steam, electricity), waste and other utilities (e.g., oxygen, hydrogen). The model is based on public information (reports, permits, websites, and interviews with stakeholders) and is representative of the complexity of the cluster. In the second phase, which is currently in progress, we are modeling (at a similar level of detail to the baseline) novel technologies that use ACS and will then be implemented in the cluster to replace the fossil base alternative to identify and evaluate potential cascading impacts. We started by focusing on one chemical building block (ethylene) and one downstream derivative (MTBE). For ethylene, from 69 potential ACS routes that were identified, 3 were selected for further modeling: direct electrochemical conversion of CO2 to ethylene; biomass steam gasification combined with Fischer Tropsch and PE low-temperature pyrolysis. For MTBE, there are less ACS routes available, and a biomass-to-isobutanol-to-MTBE synthesis process was selected. For both chemicals, we assess KPIs at the value chain and cluster level (e.g., carbon use efficiency, change in energy, water demand and cluster structure). The project generates insight into the resource, energy and costs impacts of defossilizing multiple and interconnected value chains.

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Other Authors: Amsalia Barus, TU Delft; Nikolaos Kalmoukidis, TU Delft; Savvas Staikos, TU Delft; Pieter Swinkels, TU Delft

Title: **[L54] Wind Turbine Blade Recycling Process Which Fits The Circular Economy System Concept**

Abstract: Turbine waste is expected to increase in the near future due to wind power supply growth. Currently, turbine blades are decommissioned by either landfilling or incineration: emission-intensive methods that are misaligned with the EU's sustainability policy. These blades are made of thermoset composites, which provide the necessary performance but also prevent from easily recycling back to blades. In this work, an alternative process and supply chain concept was designed using the Delft Design Map methodology, and inspired by information recently published by TNO [1] to valorize these materials with a focus on circularity. With this process, the composite fibers are recovered, and thermoplastic composites are fabricated, which unlike thermosets, can be melted and reused cyclically. The process was divided into three main segments: blade waste collection, thermoset composite processing and fabrication of thermoplastic components, in a continuous operation. Pyrolysis was selected for fibers recovery due to its technology readiness and scale-up flexibility. Caution was provided to the conditions of pyrolysis to prevent severe degradation of the fibers. The main subprocesses considered were, in sequence, on-site size reduction, transportation to plant, drying, pyrolysis, char oxidation, and extrusion/pelletization of the recovered fibers with a polyamide matrix. A preliminary market and economic analysis suggests that a plant capacity of 10 kta in the Groningen area would be feasible and entail a total energy requirement of 14 MJ/kg of feedstock, a total investment of 8.3 M€ and operational costs of 18.2 M€/yr. With a revenue of 31.4 M€/yr the project shows a positive margin and an IRR of 71% over 10 years. These financial results assume a consistent supply, which means that securing steady supplier contracts, waiting for the wind market to grow enough or reducing additional logistic costs due to longer supply distances are key for the project success. Furthermore, in order to ensure that the total process can be scaled up profitably, methods for the collection and transportation of wind turbine blades must be devised and the impact of feedstock composition variations needs to be assessed. Promotion of recyclable materials through governmental funding could also help shareholders to invest in this kind of innovative technology.

[1] Van der Mijle Meijer, Ir. H.J. (2022) Recycling of wind turbine blades for market applications. rep. TNO"

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Author: Raquel Raso Roka (Universidad de Zaragoza)

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Title:

[L55] Production of 1,2-propanediol by the aqueous phase hydrogenolysis of glycerol without external hydrogen addition over Ni/Al3Fe1: effect of the calcination temperature

Abstract:

Nowadays, the high production of biodiesel is due to the increase in environmental concerns and the exhaustion of reserves of fossil fuels. However, the output of this biofuel generates a surplus of glycerol as a by-product that could negatively affect its economy because, for every 10 tons of biodiesel, around 1 ton of glycerol is produced. In this context, it is necessary to valorise the by-product to improve biodiesel’s economy, obtaining a more sustainable process. In the biorefinery context, the aqueous phase hydrogenolysis of glycerol without external hydrogen addition (APH w/o H2) is a promising process to get a value-added product such as 1,2-propanediol (propylene glycol), which is an important chemical used in cosmetics, pharmaceuticals and among other applications. The APH w/o H2 is a catalytic process performed at moderate pressures of around 34 bar and relatively low temperatures of around 227 ºC, obtaining gas and liquid products. In addition, it is a less expensive and safer process than the conventional aqueous phase hydrogenolysis. Therefore, the present work studied the effect of the calcination temperature on the properties and performances of Ni/Al3Fe1 catalyst in the APH w/o H2 of glycerol. The Ni/Al3Fe1 catalyst was prepared by the co-precipitation method at 28 molar % of Ni and a molar ratio of Al/Fe of 3/1. The prepared catalyst was calcined at different temperatures (500-750 ºC). The obtained samples were tested in a laboratory-scale continuous feeding system (Process Integral Development Eng & Tech, Spain) which mainly consisted of a stainless steel fixed-bed reactor with an inner diameter of 9 mm and a micrometric valve which regulated the system pressure. The gas products (hydrogen, methane, carbon dioxide, carbon monoxide, ethane, and propane) and nitrogen (internal standard) were analysed online by an Agilent 490 micro-GC equipped with Thermal Conductivity Detectors (TCD). However, the liquid products (methanol, ethanol, acetol, acetic acid, ethylene glycol and 1,2-propanediol) and 1-butanol (internal standard) were analysed offline by an Agilent 7820A GC equipped with a Flame Ionization Detector (FID) and an HP-FFAP Agilent 19091F-105 capillary column. Furthermore, the prepared catalysts were characterised by various techniques (ICP-OES, XRD, H2-TPR, STEM, TGA, FESEM, NH3-TPD, N2-physisorption, and elemental analysis) before and after their use in the APH w/o H2 of glycerol. The catalyst calcined at 625 ºC was selected as the best sample due to its high catalytic activity for the 1,2-propanediol production, acidity, and metal dispersion.

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Author: Jisiwei Luo (TU Delft)

Other Authors: Mar Pérez-Fortes, Adrie Straathof, Andrea Ramirez

Title: **[L56] Optimal scheduling and sizing for a microbial electrosynthesis plant integrated with renewable electricity**

Abstract: In the context of reducing carbon emissions in the chemical industry, new technologies combining CO2 electroreduction and intermittent renewable electricity usage are emerging. Among those, microbial electrosynthesis (MES) is gaining attention, as it allows the production of high-value-added products from CO2. An interesting product from this route is hexanoic acid, which has a growing market demand and high market value. Hexanoic acid is currently a by-product of palm kernel or coconut oil production. This route is, however, strongly dependent on finite natural resources such as land and consequently, its sustainability is questioned. Featuring the potential to reduce CO2 emissions, high market value and demand, and savings on natural resources, producing hexanoic acid using a combination of MES and renewable electricity is attractive. However, the fluctuating electricity generation will impact the design of the system and the associated costs. To buffer these fluctuations, batteries and storage tanks are usually considered. Optimal sizing and efficient utilisation are expected to maximise the benefit of such a MES-based plant. The aim of the current study is then to optimise the size of the buffering units and the operating modes of the novel MES-based plant, and to assess the trade-offs between flexibility and economic performance.
We first designed and simulated a commercial-scale MES plant in Aspen Plus. The plant powered by constant grid electricity has a nominal production of 10 kt/y of 99 wt% hexanoic acid. Its levelized product cost (LPC) was estimated at 3.6 k€/t. In the second step, the plant's volume flexibility was assessed using the process model, showing that it could be operated between 70% and 100% of its nominal throughput rate without sacrificing product characteristics or damaging the process equipment. The plant was then coupled to an intermittent renewable electricity profile using Python. The LPC increased to 4.7 k€/t as a consequence of shutting downs when the minimum electricity demand for operation (i.e. 70% of its nominal throughput) was not satisfied. To reduce shutdown time, batteries and storage tanks were introduced in the model in an explorative case study, with a pre-defined plant scheduling, and pre-defined sizes for the batteries and storage tanks. The results did not favor the installation of batteries and showed that the single use of storage tanks lowered the LPC to 4.4 k€/t. Therefore, only the storage tank was incorporated into the subsequent optimisation. According to the preliminary results, the optimal storage capacity and operating modes did not lower the LPC. However, the plant can produce hexanoic acid at a larger electricity supply range, between 61% and 100% of plant's nominal electricity consumption.

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A.M. Schweidtmann, Delft University of Technology

Title: **[L57] Physics-informed reinforcement learning for process design**

Abstract: Process design is a creative task that is performed manually by engineers. Artificial intelligence (AI) provides new opportunities to facilitate process design. Very recently, reinforcement learning (RL) has shown promising results for process design [1-7]. Therein, an RL agent learns to design (bio-)chemical processes through interaction with an environment, e.g., process simulation software. However, current RL methods for process design are lacking prior engineering knowledge. Thus, they are unable to discover general physics-related concepts and transfer the gained information to new processes. We propose to incorporate physical knowledge into RL for process design. This will enable the RL agent to learn general physics-related concepts that can be transferred to different process design tasks. Specifically, we extend the current RL agent by including thermodynamic knowledge through an additional encoder architecture. We apply our novel RL agent to multiple separation case studies to demonstrate the advantages of our physics-informed RL for process design.

References

[1] Midgley, L. I. (2020). Deep Reinforcement Learning for Process Synthesis. arXiv preprint arXiv:2009.13265.
[2] Khan, A., & Lapkin, A. (2020). Searching for optimal process routes: a reinforcement learning approach. Computers & Chemical Engineering, 141, 107027.
[3] Göttl, Q., Grimm, D. G., & Burger, J. (2022). Automated synthesis of steady-state continuous processes using reinforcement learning. Frontiers of Chemical Science and Engineering, 16(2), 288-302.
[4] Fantke, P., Cinquemani, C., Yaseneva, P., De Mello, J., Schwabe, H., Ebeling, B., & Lapkin, A. A. (2021). Transition to sustainable chemistry through digitalization. Chem, 7(11), 2866-2882.
[5] van Kalmthout, S. C., Midgley, L. I., & Franke, M. B. (2022). Synthesis of separation processes with reinforcement learning. arXiv preprint arXiv:2211.04327.
[6] Sachio, S., Mowbray, M., Papathanasiou, M. M., del Rio-Chanona, E. A., & Petsagkourakis, P. (2022). Integrating process design and control using reinforcement learning. Chemical Engineering Research and Design, 183, 160-169.
[7] Stops, L., Leenhouts, R., Gao, Q., & Schweidtmann, A. M. (2022). Flowsheet generation through hierarchical reinforcement learning and graph neural networks. AIChE Journal, e17938."

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Title: **[L58] Optimization of a Membrane Cascade for Binary Gas Separation under Uncertainty of Membrane Properties**

Abstract: Separation of gas mixtures is an expensive unit operation in chemical processes that is mostly done by energy-intensive cryogenic distillation, absorption, adsorption, or a membrane gas separator (de Haan et al. (2013)) which is less energy-intensive compared to cryogenic distillation. However, membrane gas separation has an inherent trade-off between the selectivity (product purity) and the permeability of the membrane (the production rate), denoted as the Robeson upper bound (Robeson (2018)). Moreover, these membrane characteristics are often uncertain due to non-uniformity or defects of the membrane during the manufacturing process. Measurement errors during membrane characterization also contribute to parameters' uncertainty. Therefore, it is important to consider the uncertainty of membrane selectivity and permeability during the design and optimization of membrane gas separators to ensure the reliability of the process. The objective of this work is to design a membrane separation cascade for binary gas separation while considering the uncertainty of membrane characteristics by robust optimization, i.e., the worst-case scenario. In addition, the operating range where a membrane gas separator or other separation techniques is the most suitable for a specified application is identified. To reach these objectives the following steps are required; first, a model of a membrane cascade will be developed. This model consists of a superstructure, which defines connections between modules, compressors, and heat exchangers; and mass and energy balances for each unit, which consider the uncertainty of the permeability and selectivity. Second, an optimization procedure is developed. The optimization program consists of total annualized cost based on energy consumption and equipment sizes as the objective function, and the membrane cascade model as the constraints. The decision variables are the layout of the cascade, the number of stages, and the size of each stage. Finally, the MINLP is solved in Python by using Pyomo and the combination of an MINLP solver with GRCS algorithm (Isenberg et al. (2021)) or ROmodel (Wiebe et al. (2021)) to handle the uncertain parameters. Three gas pairs are used as case studies: H2-CH4, CO2-CH4, and O2-N2. The permeability of each gas is treated as a normally distributed random variable and the selectivity is a random variable defined as the ratio of permeabilities of two gases. A robust optimal layout for each application is generated, which is in some cases less costly than other separation methods depending on the operating range. The benefits and computation cost of robust optimization by GRCS and ROmodel compared to a deterministic scenario are presented. Thus, this work focuses on the consideration of parameters' uncertainty for optimization in the worst-case scenario while keeping a rigorous approach to the membrane cascade model.

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Other Authors: A.G.J. van der Ham; D.W.F. Brilman

Title: **[L59] Comparison of solvent and sorbent based carbon capture systems in LNG-fueled ships**

Abstract: In the maritime sector, the greenhouse emission accounts for 2.9% of total global emissions [1]. Although the renewable fuels are the idealistic way to reduce the greenhouse emissions, their production capacity is still not large enough to address the global energy demand. Onboard carbon capture (OCC) is a promising technology to counter fossil CO2 emission without affecting current logistics in the maritime sector. In this project a deep removal of CO2, down to less than 400 ppm as outlet concentration, is targeted to achieve net zero CO2 emissions in the LNG fuelled ships. Some challenges in the onboard carbon capture compared to that of land based processes include, limited availability of space, dynamic operational profile of the ship engine (affecting both to the capture efficiency and heat integration options) and the onboard CO2 storage [1]. Recently, the feasibility of OCC was investigated [2] and discusses the cost per ton of CO2 capture using solvent based technologies, capitalizing on the technology development for large scale operation in the power sector, targeting 80-90% removal. On a lower TRL level, sorbents are gaining importance as it offers a higher surface area and lower heat capacity, which will result in smaller equipment and less energy consumption[3], and are suitable for deep removal applications . A comparison between the potentials (with regards to energy consumption, equipment size etc.) and/or synergy of solvent and sorbent based technologies in context of OCC is not yet available in the literature. In this work, amine based capture agents (aqueous solutions and solid sorbents) are being investigated. The key performance parameters such as productivity, cyclic capacity and regeneration energy demand will be analyzed and compared for both solvent and sorbent based technologies. Additionally, possible options of integration of solvent and sorbent technologies will be discussed.

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Author: Qing Li (TU Delft)

Other Authors: Nagaraj Nagalingam; Aswin Raghunathan;Vikram Korede; Christian Poelma; Carlas S. Smith; Remco Hartkamp; Johan T. Padding; Huseyin Burak Eral

Title: **[L60] Process synthesis and design of intensified distillation sequences**

Abstract: Distillation is widely used in downstream fluid separation processes for (bio-based) fuels and chemicals due to its flexibility of handling a wide range of feed flow rates and concentrations, and the ability to produce high purity products. However, due to the relatively low energy efficiency and the usually large equipment scale, the separation stage is considered a key factor in determining the commercial success of (bio)refineries. Process intensification (PI) technologies (such as heat pump assisted distillation, heat integrated distillation column, and thermally coupled distillation systems including dividing wall columns) are considered of great potential to reduce the large costs of separation and purification steps and enhance the energy efficiency. Nevertheless, it is unclear which PI technologies are more suitable for different types of processes, and screening PI opportunities for process design becomes a combinatorial challenge. The problem is even more complex when separating multi-component mixtures because of the need of distillation sequences, as well as the many interconnected design degrees of freedom (DoF), for example, the change of basic separation configurations including complex column options, column pressures, reflux ratios, feed conditions, condenser types, and heat integration arrangements. To address this generic problem, this work contributes to develop a systematic approach. Firstly, the PI opportunities for a chemical process are identified via a novel PI matrix, in which the most appropriate PI techniques are selected based on the driving forces present in the process. The selected PI techniques are then implemented in an algorithm for the optimization of sequences synthesis and design. A process superstructure is proposed to represent automated sequences, in which the detailed heat exchanger network (HEN) design (rather than using Pinch Analysis) for heat integration is achieved through an incidence matrix. The overall optimization is formulated as a mixed integer nonlinear programming (MINLP) problem and targets to the minimum total annualized cost. An industrially relevant case study, the zeotropic mixture separation of light hydrocarbons (C2-C5+), is used to demonstrate the developed approach. Shortcut distillation methods are used for screening possible designs, and more detailed examination through rigorous simulations of the selected promising PI designs and the separation sequences is then carried out. It has been found that the sequences of light hydrocarbons separation can be screened reliably via shortcut distillation models, and the most promising distillation sequences are proposed, in conjunction with the column designs and the synthesis of heat exchanger network designs. Comparing to the conventional process, the intensified process achieves significant energy savings (over 35%). Finally, the developed process is evaluated techno-economically considering also key sustainability metrics.

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Author: Paulina A. Sosa Fernandez (UTwente)

Other Authors: Harmen J. Zwijnenberg, University of Twente

Title:

[L61] Purification of CO2-based lactic and glyoxylic acids using membrane technology

Abstract:

Global warming and carbon dioxide capture are two of the most pressing issues of this century. Once the CO2 is captured, either from industrial processes or directly from the air, it can be either directly used (for example in greenhouses), stored, or more promising; transformed into useful chemicals. Within this context, the European project CATCO2NVERS aims to develop five catalytic technologies to transform captured CO2 into useful chemicals. The chemicals were carefully chosen based on their potential usefulness in the cosmetics and plastic industry. Since one of the aims of the project is the sustainable production of these chemicals, their downstream processing is also designed for sustainability. Aiming for an electrified industrial society, membrane technology is one of the preferred options to achieve the recovery of the CO2-based chemicals. In this work, we will present the experimental work performed to recover enzymatically-produced lactic acid and electrochemically-produced glyoxylic acid. For the lactic acid case, the feed contained a mixture of other carboxylic acids, sugar, alcohol and salts, which make the purification work one of the most challenging in this project. In order to achieve the purity goal of 95%, the separation consists of several steps, including the use of electrodialysis and nanofiltration. Both technologies have been experimentally tested in the laboratory, making use of commercially available membranes. On contrast, the glyoxylic acid feed consisted only in a mixture of organic acids, which were split also using electrodialysis. At the end of the processes, lactic and glyoxylic acid with a high purity have been obtained, which brings the use of CO2-based chemicals closer to application.

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Author: Hans David Wendt (UTwente)

Other Authors: Antoine Kemperman, University of Twente; Walter van der Meer, University of Twente/Oasen; Rob Lammertink, University of Twente

Title: **[L62] A hybrid hollow fiber nanofiltration process for organic micro-pollutant removal from wastewater**

Abstract: The increasing concentration of organic micro-pollutants (OMPs) in water poses a threat to both the environment and human health. Hollow fiber nanofiltration (HF-NF) membranes have shown great potential for the removal of OMPs from wastewater effluent. We propose to recirculate the concentrate stream of a commercially available HF-NF membrane towards the preceding biological treatment of wastewater to increase the removal of OMPs. We investigated the total removal of a bioreactor combined with the HF-NF membrane, and the effect of recovery and membrane configuration on the retention of OMPs. This was done in a continuously operated pilot system at 1 m3/h, currently without concentrate recirculation. We analysed 11 OMPs with LC-MS, varying in size, charge and chemistry. The removal in the biological step varied from -20% (carbamazepine) to 99% (caffeine), with an average bioremoval of 47%. We found the highest membrane process retention for the lowest measured recovery of 70%. At this recovery, a higher process retention was obtained for a Feed&Bleed-configuration (FB) compared to a Christmas-Tree-configuration (CT). The CT-configuration outperformed the FB-configuration at 90% recovery however, because the majority of CT-permeate is created at relatively low recovery. A high NF retention is important to obtain high combined removal for OMPs with a low bioremoval, such as carbamazepine. The membrane retention of carbamazepine was 58%, leading to a small improvement in projected combined removal. The combined removal increases substantially for OMPs with a high membrane retention and a moderate biological removal, such as amisulpride, with 38% bioremoval and up to 85% retention. The projected combined removal is above 80% with concentrate recirculation, based on a a projection including the accumulation of OMPs in the recirculation loop. More than 80% is in line with targeted removals by governments, in this case more than doubling the total removal by adding the HF-NF, without the creation of a waste stream. This makes it worthwhile to experimentally investigate the concept with concentrate recirculation, including the effect of the concentrate on the biological reactor.

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Author: Qi An (TU Delft)

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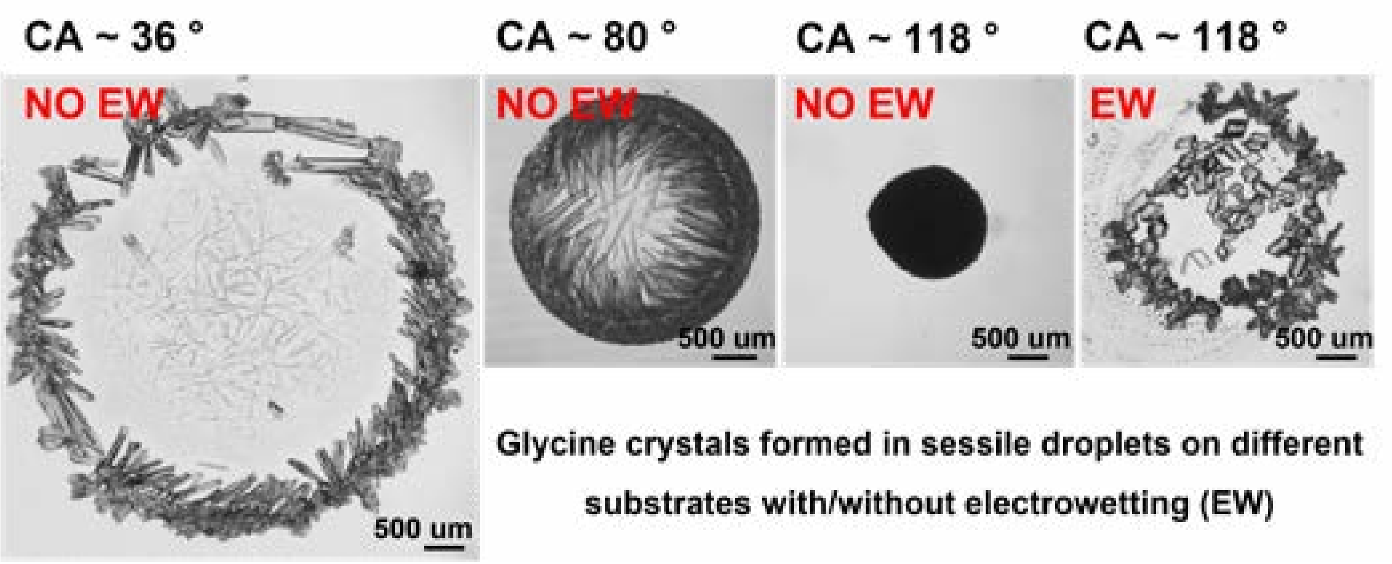
Title: **[L63] Evaporative crystallization of sessile droplets using electrowetting**

Abstract: We study the evaporative crystallization of sessile droplets of aqueous glycine solution on substrates with different contact angles, and characterize the morphologies and polymorphs of glycine. On a hydrophobic surface, the droplets evaporated without contact line pinning, and small bipyramidal α crystals formed. On a hydrophilic surface, a mixture of bipyramidal α and needle-like β crystals was observed in the coffee stain. Further, we tune the surface wettability through electrowetting, thereby achieving control over glycine crystallization. We show that electrowetting is promising for customized crystallization.



Glycine crystals formed in sessile droplets on different substrates with/without electrowetting (EW)

000076-Q-evaporative-crystallization-of-sessile-droplets-using-electrowetting.png

Author: Jose Palomo Jimenez (TU Delft)

Other Authors: Noah Koenraadt, TU Delft; Jim de Kort, TU Delft; Atsushi Urakawa, TU Delft

Title:

[L64] Operando spatial reactor analysis for the kinetic study of oxidative coupling of methane

Abstract:

Natural gas reserves and shale gas exploitation ensure availability of methane in the next decades and centuries, making this compound a potential substitute to crude oil for light olefins production provided feasible methane upgrading processes can be developed. Oxidative Coupling of Methane (OCM) is a direct and exothermic process offering a straightforward pathway for the conversion of methane into value-added chemicals, such as ethane and ethylene. However, due to the high temperatures required for methane activation (higher than 700 ºC), deep oxidation reactions also take place in the process, which lower the yield towards the desired C2+ products. In the last decades, a huge effort was made in the development of new and efficient catalysts. On the other hand, the number of studies dealing with understanding OCM reaction mechanism and kinetics is limited. OCM proceeds through a complex radical-mediated homogeneous (gas phase) -heterogeneous (surface) reaction network. In addition, the presence of both endothermic and exothermic reaction step in OCM usually results in the apparition of temperature gradients in the catalyst bed. This intrinsic complexity makes the elucidation of comprehensive kinetic models a challenge. In this work, we present an experimental methodology based on the use of operando spatial reactor analysis techniques. This experimental approach was used to gain insights into the OCM reaction mechanism on La2O3 and MgO catalysts. Spatially resolved temperature and concentration profiles under operando conditions, were obtained using a customised reactor system that allows gas sampling and temperature measurements at different axial positions (<1 μm precision). A thermal infrared camera was also used to determine the presence of hotspots and localised thermal phenomena in the catalyst bed. IR thermography images of the catalyst bed showed temperature deviations as high as 100 ºC, evidencing the importance of these physical phenomena in the OCM process. Catalyst dilution with SiC particles was used as a means to influence/control the magnitude of the thermal gradients present in the catalyst bed. Even at high catalyst dilution ratios, Cat:SiC = 1:15, considerable temperature deviations from the reaction temperature were observed (See Figure 1). Spatially resolved concentration profiles along the reactor were determined for reactants and products (See Figure 2). A comprehensive kinetic model, accounting for the homogeneous-heterogeneous nature of the OCM, was developed for the OCM process. This model includes 39 gas phase reactions and 8 elementary heterogeneous surface reactions. Kinetic and thermodynamic parameters for the heterogeneous elementary steps were estimated. A rate analysis was carried out, being it feasible to estimate the importance of both the heterogeneous and homogeneous reactions in the overall OCM process.

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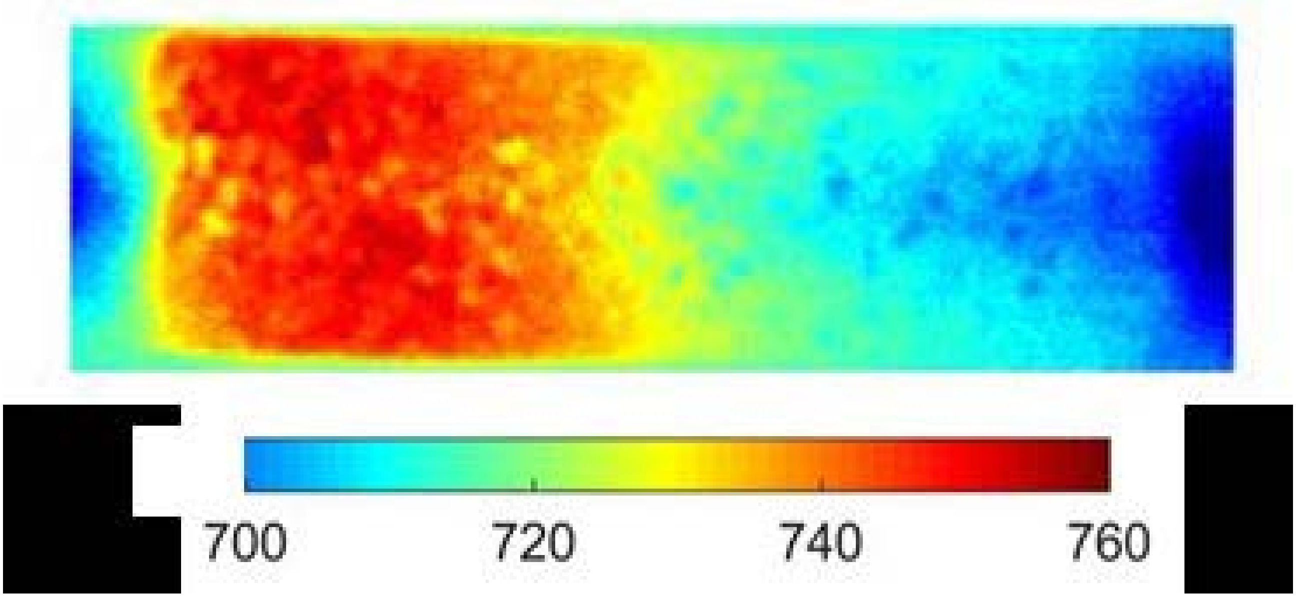

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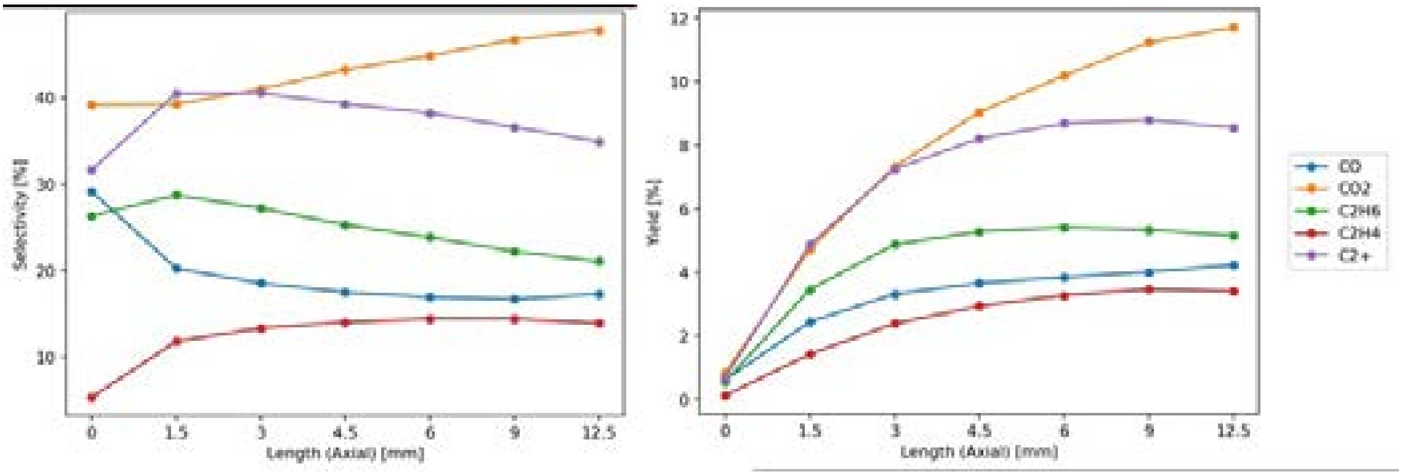

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Author: D.R. (David) Rieder (TU/e)

Other Authors: E.A.J.F. (Frank) Peters; J.A.M. (Hans) Kuipers

Title: **[L65] Precipitation of species during drying in catalyst preparation**

Abstract: Porous media are widely used materials in process engineering, e.g. as filters or catalyst supports. Among their key characteristics, the high specific surface area is commonly exploited in order to significantly increase the contact area between fluid and solid. Especially in the field of heterogeneous catalysis, this high contact area is of critical importance to the final performance of a reactor. Additionally, the spatial distribution of the commonly used catalytically active precious metals within the support structure is a key factor for a successful economic operation of the target process. However, industrial production of such heterogeneous catalysts often involves impregnation, drying and subsequent calcination, where the deposition location is highly dependent on the hydrodynamics within the porous media. Especially drying has a major impact on the final distribution of the waterborne active species. There, capillary-force induced hydrodynamics introduce a significant redistribution of liquid within the pore system. Additionally, in the case of relatively high precipitate volumes, the introduced change in pore size geometry leads to an intricate interplay between capillary and viscous forces. Therefore, an in-depth understanding of the redistribution process, as well as its behavior within a continuously changing geometry due to industrially relevant deposit loads is required to provide optimized porous structures.To better understand this phenomena we have developed a particle scale model based on Darcy-type of flow, taking into account the relevant heat and mass transfer mechanisms. Additionally, we introduced a capillary model that enables the computation of the hydrodynamic properties of the porous media from arbitrary pore size distributions. Within this presentation, we highlight a precipitation model coupled to the computation of the hydrodynamic properties and its impact on post-drying distribution of the precipitate.

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Author: Zhuo Zhang (UTwente)

Other Authors: Srinivas Vanapalli, University of Twente; Midhun Joy, Air Liquide Innovation Campus

Title: **[L66] Solidification and Solute Redistribution During a Progressive Freeze Concentration Process -Theoretical Modeling and Experimental Validation**

Abstract: The Progressive Freeze Concentration (PFC) process enables a gradual removal of water content present in a liquid solution in the form of ice, resulting in a concentrated liquid phase with an elevated solute concentration. The overall efficiency of a PFC process is expressed in terms of the averaged partition coefficient (K), which represents the ratio of the average concentration of the solute in the ice and liquid phases after a PFC process. The current modeling approaches to estimate K are constrained by the limited capability to capture the impact of ice growth rates, often leading to inaccurate predictions. To overcome this limitation, a coupled heat and mass transfer model is proposed to estimate K, which considers the dynamic change of the ice growth rate and the concentration of solute in the ice and liquid phases. The developed model was also validated with PFC experimental data obtained from a lab-scale concentrator with sucrose as the solute. It was demonstrated that the proposed model could accurately capture the dynamics in the PFC process and that the total ice mass and the final liquid concentration predicted from the model agree well with the experimental data. Based on the proposed model, the cooling profile for zero solute inclusion in the PFC process is theoretically calculated, which can be used to reduce the operational costs of the system.

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Author: Abhishek Purandare (UTwente)

Other Authors: Srinivas Vanapalli, University of Twente

Title: **[L67] Sublimation temperature of carbon dioxide for varying ambient pressure and far-field concentration**

Abstract: The cooling potential of sublimating solid carbon dioxide (dry ice) is vital in applications such as spray cooling food and pharma products and cryopreservation. The thermodynamic saturation temperature of solid carbon dioxide at normal atmospheric pressure is -78.5 ºC. Application engineers often use this temperature data to design cooling equipment without noticing that this temperature refers to the phase change process between the solid and vapor carbon dioxide. In the air, due to nearly zero far-field concentration of carbon dioxide, the diffusion of carbon dioxide vapor from a sublimating dry ice surface will decrease its internal energy, causing a further decrease in the sublimation temperature. We measured the temperature of a dry ice sphere in a climate chamber where the far-field concentration of CO2 and the absolute pressure is varied. This data is compared with a transport model that includes thermal and mass diffusion. This model predicts well the steady state sublimation temperature of the dry ice for various conditions

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Author: Gaetano Anello (TU/e)

Other Authors: Arash Rahimalimamaghani, TU/e; Luca Di Felice, TU/e; Fausto Gallucci, TU/e

Title: **[L68] Ru-based nanocatalysts for ammonia production in Membrane Reactors**

Abstract: Hydrogen can be considered as an ultimate clean fuel, as the only product obtained from its combustion is water. Still, the transport and storage of hydrogen in any form are an issue due to the risks related to its wide flammability range and low ignition energy. A safe way to store hydrogen is through a suitable carrier: ammonia is an interesting solution as in the liquid form provides a high hydrogen density and the infrastructures involved in its production, storage and distribution are already fully operating. In the last decades, Ru-based catalysts have emerged as second generation catalyst for NH3 synthesis, due to the higher activity at lower temperatures and pressures than conventional catalysts [1]. However, Ru-based catalysts have two main drawbacks: high cost and hydrogen poisoning [2]. Therefore, to increase the performance of Ru-based catalysts, the focus of this research is the maximization of the catalytic activity through the maximal exposure of ruthenium active sites. Moreover, the equilibrium constraint of this reversible reaction can be overcome by removal of the reaction product thanks to a selective membrane. Ruthenium-based Ba-promoted catalyst has been prepared by polyol reduction method. Magnesium nitrate hexahydrate, ruthenium chloride and barium nitrate have been dissolved in pure ethylene glycol under nitrogen atmosphere and vigorous stirring. After the saturation of the reflux column, a heating mantle has been used to heat-up the solution to 110°C for 120 min giving a dark colloidal solution. The resultant gel was aged for 10 min and submitted to five cleaning cycles by deionized water. Then, the gel was dried and then calcined at 500°C. Ba-Ru/MgO catalyst prepared was characterized trough XRD (Image 1). In the XRD pattern only the characteristic peaks of MgO can be observed. These peaks at 36.9°, 42.9°, 62.3°, and 78.6° can be attributed to the (111), (200), (220) and (222) planes of magnesium oxide (JCPDS card no. 45-0946) [3]. No diffraction features assignable to ruthenium and barium could be identified and this suggests that the crystal size of these particles was too small to be detected. As evidenced by the TEM images of the sample (Image 2), the Ru particles are homogenously distributed throughout the MgO support. The well-dispersed feature is the result of the mild reduction process by ethylene glycol. Furthermore, the actual metal loading was measured with ICP-OES: it was found that the loading was respectively 3%wt for ruthenium and 1%wt for barium.The catalytic behavior of the catalyst will be tested in a membrane reactor in combination of carbon membranes. The high activity of the catalyst synthesized together with the removal of the reaction product thanks to the porous structure of the membrane, might enables an efficient ammonia synthesis and separation under mild conditions.

[1] 10.1021/ja031718s : [2] 10.1016/j.jcat.2020.06.037 : [3] 10.1039/d0nj03157g”

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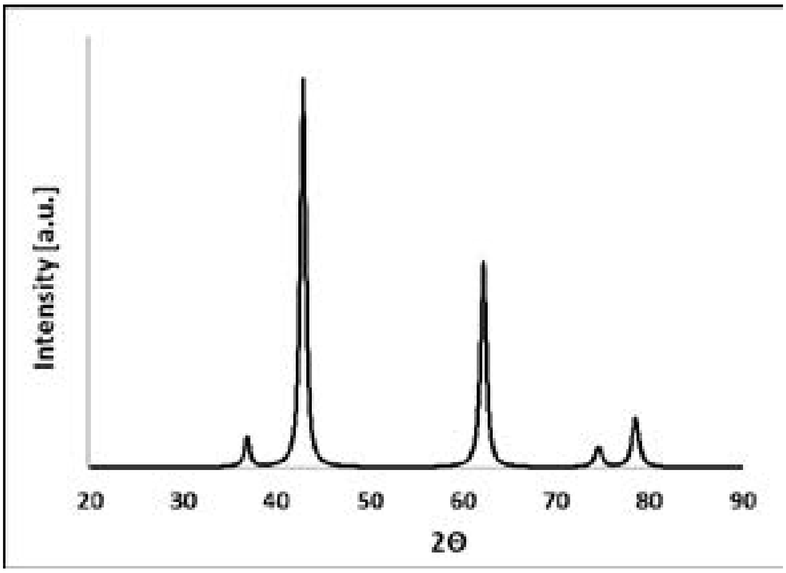

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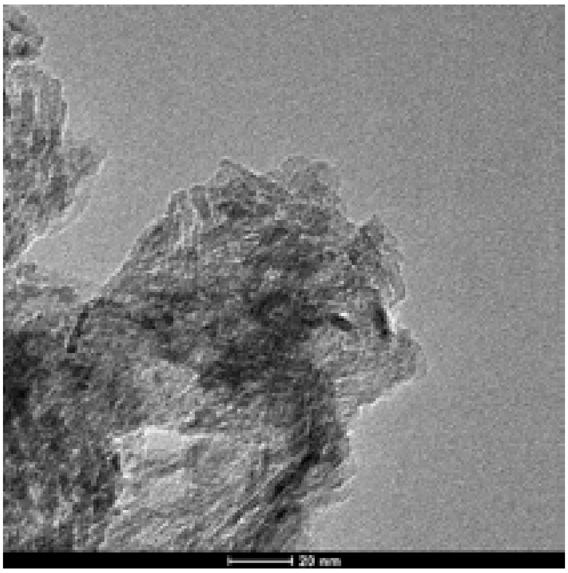

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Author: Mert Can Erer (TU/e)

Other Authors: Antoni Forner-Cuenca, TU/e

Title: **[P01] Designing Gas Diffusion Electrodes with Tailored Wettability for CO2 Reduction Electrolyzers**

Abstract: Pressing environmental issues and climate change motivates the decarbonization of the energy economy and the chemical industry. To this end, the carbon dioxide (CO2) electrolysis has emerged as an attractive negative-carbon technology to produce valuable chemicals such as ethanol and ethylene. In recent years, gas diffusion electrodes have been introduced to achieve higher current densities by improving mass transport rates and eliminating the challenge of large diffusion lengths and low CO2 solubility in water persistent in liquid electrolytes.[1] A gas diffusion electrode is composed of two components, the gas diffusion medium and the catalyst layer. Commercial diffusion media consists of two sub-layers, a macroporous carbon fiber substrate and a finer porosity layer of carbon nanoparticles, namely the microporous layer, which are hydrophobized with a fluorine-based polytetrafluoroethylene (PTFE) coating[2]. Insufficient electrolyte/product repellency by the surface results in catastrophic flooding of the electrode, dramatically reducing the operational time of the reactor. Although the PTFE-coated diffusion media might provide sufficient hydrophobicity for water, they fail to prevent the infiltration of low surface tension (≈ 22 mN/m) liquid products, such as ethanol,[3] which motivates the development of alternative coating chemistry for enhancing the reactor stability. Within this scope, while previous research efforts have investigated the effect of wettability on the catalyst layer[4], the impact of wetting on the diffusion medium remains largely unexplored. In this study, we explore the application of oleophobic coatings with low surface energy on the diffusion medium.
To this goal, non-fluorinated chemistry will be employed to eliminate the negative environmental impact of the fluorine utilization. The wettability of the coated substrates will be characterized through static and dynamic contact angle measurements, probing the surfaces using water and the liquid organic products of CO2 electrolysis. The structural and morphological analyses of the developed coatings will be performed via spectroscopy and microscopy. We hypothesize that surface chemistry of the diffusion media could be tailored to impart oleo/hydrophobicity that could potentially surpass the PTFE coated commercial materials and enhance the reactor performance for CO2 electrolysis by suppressing electrode flooding.

References

[1] Z. Xing, L. Hu, D. S. Ripatti, X. Hu, X. Feng, Nat Commun 2021, 12, 136.
[2] E. W. Lees, B. A. W. Mowbray, F. G. L. Parlane, C. P. Berlinguette, Nat Rev Mater 2021, 7, 55.
[3] M. E. Leonard, M. J. Orella, N. Aiello, Y. Román-Leshkov, A. Forner-Cuenca, F. R. Brushett, J. Electrochem. Soc. 2020, 167, 124521.
[4] M. Li, M. N. Idros, Y. Wu, T. Burdyny, S. Garg, X. S. Zhao, G. Wang, T. E. Rufford, J. Mater. Chem. A 2021, 9, 19369.

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Author: Rick Baldenhofer (UTwente)

Other Authors:

Title: **[P02] The conversion of furfural to bio jet fuel**

Abstract: Due to the increasing scarcity and environmental impact of fossil-based fuels, it is becoming very important to search for renewable alternatives. One of the platform chemicals identified to play a key role in the energy transition is furfural. Furfural is an important precursor for the production of jet fuel ,among others, and it can be produced from lignocellulosic biomass. Many different routes for the upgrading of furfural to fuels are known. These routes are often novel routes which have not yet been fully explored or developed. Therefore, challenges arise in its large scale production. In this context, the interest of this project is to explore potential routes for the large scale production of jet fuel from furfural. Different approaches have already been discussed in literature, but most of them lack a cyclic component needed to provide adequate combustion and freeze point properties. A promising route to consider is via aldol condensation reaction of furfural with cyclopentanone. A sequential hydrogenation reaction will yield a promising feedstock for further upgrading towards replacement and blend in bio jet fuels. The focus off the project lies on exploring the integration and intensification of the various processing steps and developing means to accommodate higher concentrations and productivity to avoid complex work-up of intermediates to be transferred between steps.

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Author: Jesse Thomas Benjamin de Boer (TU/e)

Other Authors: Antoni Forner-Cuenca,TU/e

Title: **[P03] Surface functionalization of Cu electrocatalysts for the electrochemical reduction of CO2 to ethylene with improved selectivity and durability**

Abstract: Converting greenhouse-contributing CO2 into valuable products is a promising route to reduce the concentration of CO2 in the atmosphere. To this goal, the electrochemical CO2 reduction reaction (eCO2RR) with Cu-based catalysts can support the decarbonization of the industrial production of commodity chemicals owing to the possibility to synthesize a wide variety of C2+ products in a carbon neutral way.[1,2] In particular, ethylene is highly valued for industrial uses, including chemical precursors, polymer fabrication, and fuel for energy generation. The production of ethylene with the eCO2RR involves a multi-step electron and proton transfer process, which inevitably leads to the formation of by-products. Currently, the eCO2RR suffers from low product selectivity and lacks in catalyst stability to be viable at large scale.[3] In this project, we will develop new types of electrodes to improve the selectivity towards ethylene production and the reactor stability. To that end, we will use Cu-based catalysts owing to its ability to produce products beyond CO.[4] It has been reported that the incorporation of polymers on Cu-based catalyst electrodes improves the overall stability of the catalyst and influences the binding energies of CO2 intermediates absorbed on the Cu-sites.[5,6] The latter has a positive influence on the electrochemical reduction of CO2 towards C2+ products. However, the polymer films have been mainly deposited by dip coating or drop casting techniques which do not enable precise control of the coating thickness, morphology, and distribution. To accurately control the thickness and morphology of the coated polymer layer, we will deploy electropolymerization of selected monomers with electron donating properties. Altering the thickness and morphology of the polymer coatings influences the local environment of the catalyst layer, providing an additional handle to tune product selectivity in eCO2RR. By comparing the different polymer coatings and accurately tuning the coating thickness and morphology, we aim to increase the eCO2RR selectivity towards the production of ethylene. This work on copper-modified catalysts will be combined with gas diffusion electrode substrates and tested in flow cell setups. Eventually, we hope that this research will help to scale-up CO2 electrolysers to accelerate the transition to a sustainable production of ethylene.

References:

[1] P. De Luna, C. Hahn, D. Higgins, S. A. Jaffer, T. F. Jaramillo, E. H. Sargent, Science 2019, 364, eaav3506.
[2] R. Kortlever, J. Shen, K. J. P. Schouten, F. Calle-Vallejo, M. T. M. Koper, J. Phys. Chem. Lett. 2015, 6, 4073.
[3] L. Fan, C. Xia, F. Yang, J. Wang, H.

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Title: **[P04] On the influence of trialkylamine reduction strategies in the direct hydrogenation of CO2 to formic acid**

Abstract: Formic acid is often seen as a promising organic molecule to store hydrogen, as it readily allows for a reversible transformation back to hydrogen and CO2 besides being a valuable bulk chemical for preservatives and antibacterial agents [1]. Formic acid is known to store 4.3 wt% hydrogen and is liquid at ambient conditions, therefore allowing straightforward storage and transport [1]. Even though the state-of-the-art catalysts seem sufficiently active and selective [1][4][5], the equilibrium concentrations reached remain low due to the reaction being thermodynamically unfavorable [4]. Promising results have been obtained using tertiary alkylamines [6][7]. While promising results were obtained for triethylamine (NEt3) in previous works [6][7], the formed salt does not allow for direct thermal splitting [6][8]. Low-boiling amines such as NEt3 result in stable azeotropes, rendering separation through (vacuum) distillation impossible, thereby significantly complicating separation processes [6]. Previous works have shown that the usage of NHex3 (trihexylamine) allows for thermal cleavage under mild conditions (150 -, 150 mbar) [8], therefore enabling the formic acid to be readily separated from the reducing agent. From here it readily becomes apparent that the ability to separate the produced formic acid and the tertiary alkylamine is crucial for the economic viability of the proposed process, providing the motivation for this work. Here, the intent is to allow for thermal cleavage of the produced adducts, while maintaining the promising yields found in previous works, such as [6][7]. To gain a deeper understanding into key reaction mechanisms, the aim is to elucidate the influence of the tertiary alkylamine hydrocarbon length on key reaction parameters such as CO2 conversion and selectivity towards formic acid. The direct hydrogenation was studied at temperatures between 35-90°C and 10-20 bar using a 1:1 volume mixture of H2 and CO2 in an autoclave together with the aforementioned amines as a reduction base, with no other solvents added. The selected catalyst is commercially available Au/ TiO2. The liquid reaction mixture is monitored using in-line 1H-NMR (Magritek, 43 MHz). The reliability of in-line 1H-NMR was verified through comparison with a high resolution 400 MHz off-line 1H-NMR. The biphasic nature of the tertiary alkylamine – formic acid system was found to have significant implications for the reaction performance of the proposed system. The inability of the adduct to dissolve in the available non-binding amine results in the catalyst pores readily reaching equilibrium, with the system unable to refresh the reagents in the catalyst pores. Initial results have shown that by removing the biphasic nature of the reaction mixture through the addition of a solvent, a significant improvement in formic acid production is obtained.

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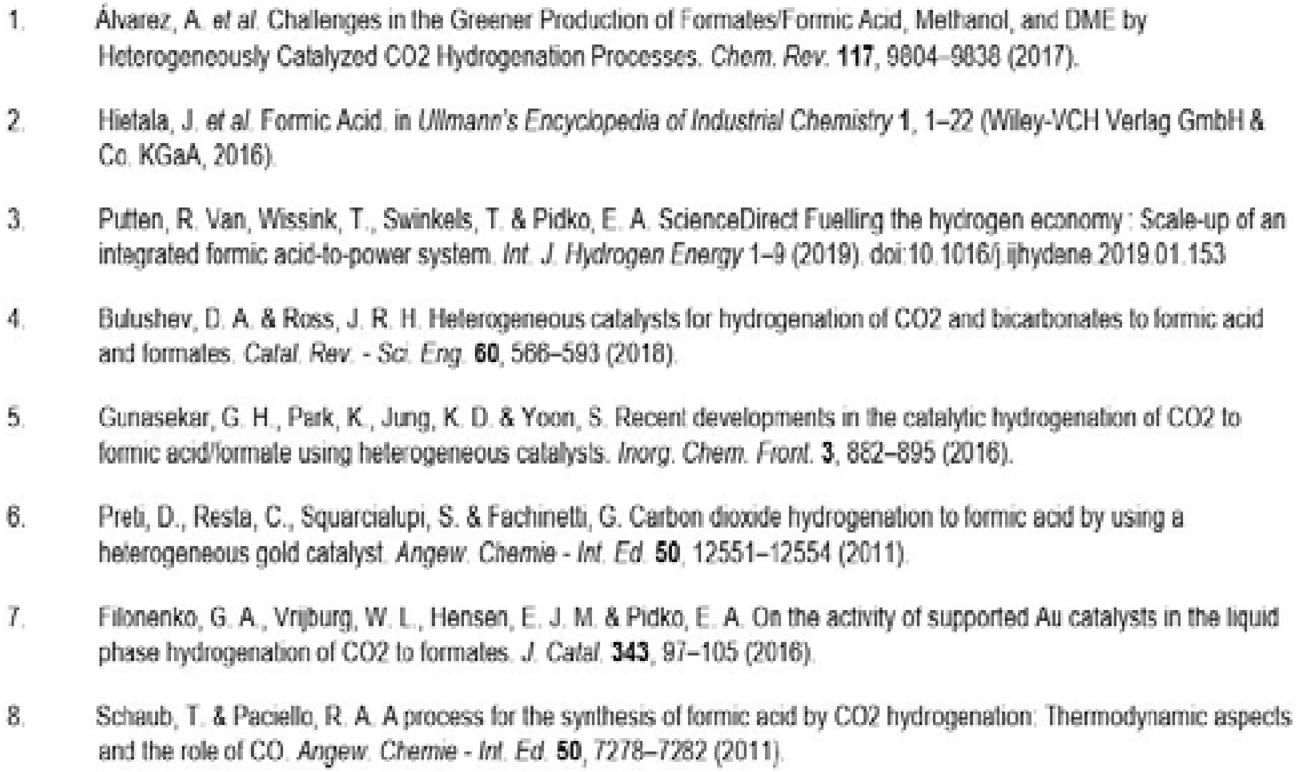

1. Álvarez, A. *et al.* Challenges in the Greener Production of Formates/Formic Acid, Methanol, and DME by Heterogeneously Catalyzed CO2 Hydrogenation Processes. *Chem. Rev.* **117**, 9804–9838 (2017).
2. Hietala, J. *et al.* Formic Acid. in *Ullmann's Encyclopedia of Industrial Chemistry* **1**, 1–22 (Wiley-VCH Verlag GmbH & Co. KGaA, 2016).
3. Putten, R. Van, Wissink, T., Swinkels, T. & Pidko, E. A. ScienceDirect Fuelling the hydrogen economy : Scale-up of an integrated formic acid-to-power system. *Int. J. Hydrogen Energy* 1–9 (2019). doi:10.1016/j.ijhydene.2019.01.153
4. Bulushev, D. A. & Ross, J. R. H. Heterogeneous catalysts for hydrogenation of CO2 and bicarbonates to formic acid and formates. *Catal. Rev. - Sci. Eng.* **60**, 566–593 (2018).
5. Gunasekar, G. H., Park, K., Jung, K. D. & Yoon, S. Recent developments in the catalytic hydrogenation of CO2 to formic acid/formate using heterogeneous catalysts. *Inorg. Chem. Front.* **3**, 882–895 (2016).
6. Preti, D., Resta, C., Squarcialupi, S. & Fachinetti, G. Carbon dioxide hydrogenation to formic acid by using a heterogeneous gold catalyst. *Angew. Chemie - Int. Ed.* **50**, 12551–12554 (2011).
7. Filonenko, G. A., Vrijburg, W. L., Hensen, E. J. M. & Pidko, E. A. On the activity of supported Au catalysts in the liquid phase hydrogenation of CO2 to formates. *J. Catal.* **343**, 97–105 (2016).
8. Schaub, T. & Paciello, R. A. A process for the synthesis of formic acid by CO2 hydrogenation: Thermodynamic aspects and the role of CO. *Angew. Chemie - Int. Ed.* **50**, 7278–7282 (2011).

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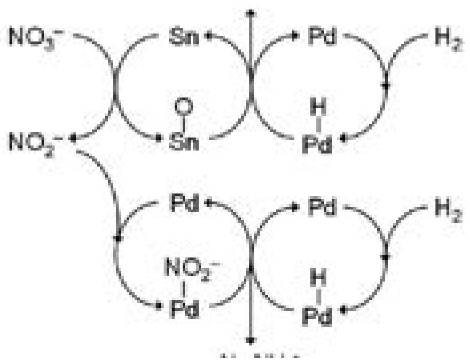
Title: **[P05] Heterogeneously SnPd-catalysed Nitrate and Nitrite reduction in aqueous solution**

Abstract: The development of a zero-emission ship engine system can reduce substantially the emissions generated from freight transport. This is very attractive in liquified natural gas (LNG) powered ships as the captured CO2 can be converted back to methane using green hydrogen, enabling the circular use of carbon-based fuels. Unfortunately, the combustion of LNG emits a so-called “methane slip” as well as NOx gases. To capture all the emissions, methane can be catalytically oxidized to CO2 and the NOx emissions can be scrubbed into liquid phase resulting in a nitrate and nitrite containing solution.[1] Converting these oxidized nitrogen species back to N2 is key to prevent the disposal of these waters into the harbors as the high concentration of nitrates and nitrites will promote eutrophication of the water bodies and aquifers near the area.It is known that bimetallic catalysts are required to convert nitrates into N2. While Pd-Cu systems are most investigated, e.g. Pd-Sn systems exhibit better performance.[2] On the other hand, monometallic catalysts based on Pd or Pt suffice for nitrite reduction. For SnPd-based systems it is assumed, that tin is oxidized to tin(II) oxide to reduce nitrate into nitrite. Palladium oxidizes hydrogen and reduces nitrite to nitrogen and also recovers tin(0) via a hydrogen spill-over mechanism (Figure[3], top). Nitrite is subsequently reduced at a Pd site with hydrogen as reducing agent. Within this reduction both N2 and ammonia can be formed (Figure, bottom). As ammonia would similarly lead to eutrophication this reaction must be suppressed. Therefore, the aim of this work is to develop, investigated and optimize heterogeneous SnPd/γ-Al2O3 catalysts regarding activity and selectivity towards N2 for the reduction of a nitrate and nitrite mixture in aqueous solution. For that purpose, we will combine detailed reaction kinetics and catalyst characterization to establish fundamentally relevant property-chemistry-performance relationships.

References:
[1] O. Ghriss, H. ben Amor, H. Chekir, M. R. Jeday, J Mater Cycles Waste Manag 2020, 22, 56–64.
[2] I. Sanchis, E. Díaz, A. H. Pizarro, J. J. Rodríguez, A. F. Mohedano, Sep Purif Technol 2021, 255.
[3] J. Hirayama, Y. Kamiya, Catal Sci Technol 2018, 8, 4985–4993.”



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Title: **[P06] Cobalt-based Fischer-Tropsch Synthesis catalysts for the conversion of CO2-rich syngas**

Abstract: Carbon capture and conversion of industrial flue gasses 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 over cobalt-based catalysts has been extensively investigated, but the conversion of CO¬2 over these type of catalysts produces mainly methane [2]. Industrial flue gases e.g. typical steelwork off-gases are mainly composed of CO, CO2, H2 and N2 and therefore a reverse water gas shift and gas separation step would be needed to convert these flue gases into synthesis gas [3]. However, if the Fischer Tropsch process would be tolerant for CO2, a one-step conversion of flue gas into long chain hydrocarbons could be achieved. The performance of cobalt-based catalysts for mixed feed Fischer Tropsch is debated as some research claims the CO2 to be an inert whereas others claim the CO2 to be hydrogenated into methane along with the CO [4,5]. Surprisingly when a 50/50 CO2/CO feed was used over a cobalt on titania P25 catalyst a C5+-selectivity of almost 80 % could be achieved. These results are difficult to compare with state-of-the-art literature because in mixed feed experiments, the ratio of H2/atomic carbon is often different which affects the conversion level and besides, an increase in CO2 content changes the H2/CO ratio which affects the CO conversion as well [6]. In Figure 1, the C5+-selectivity versus CO outlet partial pressure is given for various H/atomic carbon ratios and with a sufficient CO-partial pressure available, a high C5+-selectivity can be achieved. In this work the CO conversion level and hence the CO outlet pressure is tuned for different CO2/CO mixtures by varying the GHSV. Based on these results, the highest possible CO2-concentration in a mixed feed Fischer-Tropsch process for the efficient production of synthetic aviation fuels is determined.

Figure 1 C5+-selectivity versus CO partial pressure in the outlet for various CO and CO/CO2 Fischer Tropsch experiments with varying H2/atomic carbon ratios. The reactions are performed in a PBR at 220oC 20 barg with argon as internal standard.

[1] SkyNRG, “Sustainable aviation fuel: Technology,” 2021. https://skynrg.com/sustainable-aviation-
fuel/technology/ (accessed Dec, 2022).

[2]Fan et al. Journal of Physical Chemistry Letters 2021 12 10486–10496.

[3] W. Uribe-Soto et al. Renewable and Sustainable Energy Reviews 2017, 74, 809–823.

[4] T. Riedel et al. Appl Catal A Gen 1999, 186, 201–213.

[5] Y. Yao, et al. Industrial and Engineering Chemistry Research 2010, 49, 11061–11066.

[6] I. C. Have et al. Nat Commun 2022, 13.

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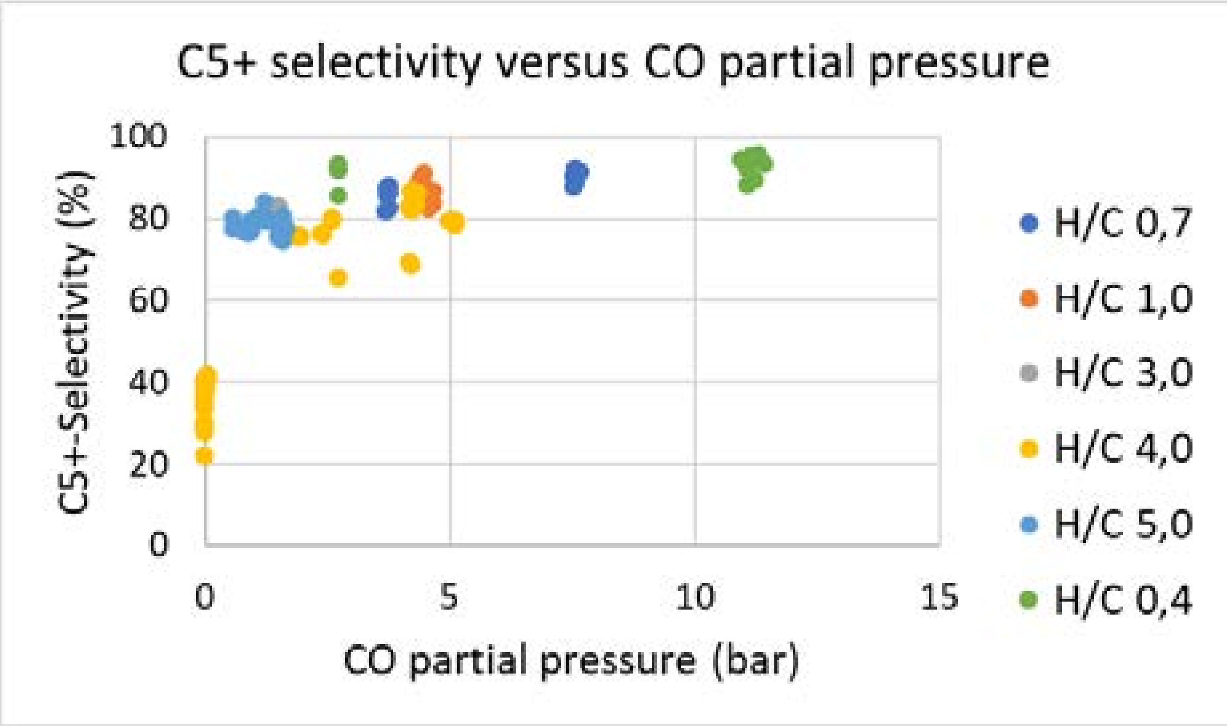

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Title: **[P07] Creating lumped models for fluidized bed gasifiers using CFD**

Abstract: Fluidized beds have been studied for multiple decades, as alternative reactors for energy conversion and fuel from a wide variety of feedstock. There are various kinds of physics that have to be studied in a fluidized bed, namely hydrodynamics, heat & mass transfer and chemical kinetics. In this light, several experimental and computational models have been defined in order to correlate the interplay of these physics. However, despite several correlations being employed, there is still a need to provide simplistic models to study the various interactions between the physics and chemistry involved. Therefore, the main aim of this PhD is to simplify interactions between these physics by creating a one-dimensional lumped model. The idea of this model is to enhance the speed of calculations. Different kinds of modelling techniques are also to be employed in order to check the feasibility of the study. The current focus is on nozzle simulations for single and double-media nozzles, to be used in the final gasifier setup. Two kinds of nozzles are to be investigated for their performance characteristics - a single medium consisting of superheated steam, and the other being a double media nozzle having oxygen and superheated steam. The following approaches have been planned:

1. Tracking particles using Bezier curves, and projecting their motion into 2D planes.
2. Comparing TFM with Dense Discrete Particle Modelling (DDPM) models.
3. Benchmarking results with different software.

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Title: **[P08] The Drive-Down System for Production, Storage, and Transport of Emission-Free Hydrogen**

Abstract: The volatility of wind and solar energy leads to electricity curtailment due to out-of-sync demand and supply. This costs electrical companies significant curtailment costs[1]. Consequently, the volatility needs to be buffered, for example, by hydro dams[2], batteries[3], or power-to-gas[3] systems. The Drive-Down (DD)1 System was developed as a model for optimization and evaluation for a production and supply system of economically competitive emission-free energy carriers2, with the following characteristics to increase the efficiency of the process:
a. Surplus solar and wind energy are stored as compressed hydrogen in lightweight vessels with compression energy recovery (DD-Vessels)[4]. b. Conversion of energy to gas and gas to energy utilizes the combination of PEMWE and PEMFC. c. Compressed hydrogen is distributed at high energy density (ca. 40 kg H2/m3) compared to, e.g., battery packs. d. The transport of hydrogen can be carried out by truck, train, or ship separate from the electrical grid. A case study based on the energy consumption of public transport buses shows DD-system competitiveness to diesel fuel. Present evaluations show that the marginal cost price of compressed hydrogen and electricity by DD-System is €2,50/kg H2 and €0,21/kWh, respectively. Production facilities are available for all elements of the system. Successful implementation is dependent on the testing and development of DD-Vessels[4].References:

[1] P. Tisheva, UK wind curtailment cost in past two years put at GBP 806m, Renewables Now. (2022)
[2] H.W. Sinn, Buffering volatility: A study on the limits of Germany’s energy revolution, Eur.Econ. Rev. 99 (2017)
[3] J. Sijm, P. Gockel, M. van Hout, Ö. Özdemir, J. van Stralen, S. Koen, A. van derWelle, J. de Joode, W. van Westering, M. Musterd, Demand and supply of flexibility in the power system of the Netherlands, 2015-2050
4] L2 Consultancy B.V., Tank And System For Storing Compressed Gas, e.g. CompressedHydrogen Vehicle; System and Method for Supplying Gas to a Tank
[5] L2 Consultancy B.V., System and method for adjusting pressure in a reservoir and system for producing at least one energy carrier
[6] L2 Consultancy B.V., System and method for adjusting pressure in a reservoir and system for producing at least one energy carrier,

Footnotes:
1 The Drive Down (DD) label of this hydrogen storage & transport system refers to the development mission of
L2C (the inventor) to achieve ‘Driving Down the Consumption of Carbon Fuels’.
2 These features are covered by the following patents: NL2024566[5], NL2025903[6]

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Title: **[P09] Digitization of Process and Instrumentation Diagrams (P&IDs) using Deep Learning**

Abstract: Engineering diagrams are essential to communicate information in the chemical industry. In particular, Process Flow Diagrams (PFDs) and Process and Instrumentation Diagrams (P&IDs) document the topology of major unit operations, control equipment, and pipes. Despite the availability of advanced CAD software, engineering diagrams are still commonly stored and communicated as PDFs, images, or printouts. Consequently, companies have huge amounts of engineering diagrams that are not machine-readable. This analog way of storing information leads to a large number of practical issues. We propose a computer vision algorithm that digitizes P&IDs and PFDs. Our algorithm consists of three steps: First, the location and type of unit operations are detected through a convolutional neural network (CNN). The CNN is trained on heterogeneous process flowsheet data gathered from different sources, and uses a pretrained object detection algorithm to identify all unit operation accurately. In addition, all tags and other text is detection through object detection and digitized through optical character recognition (OCR). In the second step, a computer vision algorithm identifies the connections, line types, and directions. Finally, we use the extracted information to generate a machine-readable graph representation of the chemical process. Our results demonstrate a high precision and robustness of the approach.

Reference

Theisen, M. F., Flores, K. N., Balhorn, L. S., & Schweidtmann, A. M. (2023). Digitization of chemical process flow diagrams using deep convolutional neural networks. Digital Chemical Engineering, 6, 100072.

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Title: **[P10] Liquid Organic Hydrogen Carriers - Process design and economic analysis for manufacturing N-ethylcarbazole**

Abstract: The production of renewable energy is often intermittent and commonly distant from the location of usage. Therefore, it is necessary to find a suitable method to store and transport the generated energy. Hydrogen has proven to be a promising candidate and is currently stored and transported either after severe pressurization [1] or cryogenic liquefaction, which consume 20-40% of the energy stored in H2 [2]. Milder conditions can be achieved with a Liquid Organic Hydrogen Carrier (LOHC) [3], i.e., by hydrogenating an organic component at the power generation site and subsequently dehydrogenating it at the usage site. Recent studies indicate prohibitive manufacturing costs for LOHC, e.g, €5/kg for dibenzyltoluene [4], resulting in large capital costs associated with transporting H2 [5]. Therefore, lowering the LOHC production costs would make its use for H2 transport and storage more viable. This research paper revisits the economics of N-ethylcarbazole (NEC) (see Fig. 1), a strong candidate for large-scale LOHC production, for its high H2 storage capacity (5.8wt%), selective hydrogenation and dehydrogenation reactions and compatibility with existing fuel infrastructure [3]. Based on an extensive literature search, two different process routes using industrial chemicals were selected: One using aniline (method 1) and the other using cyclohexanone and nitrobenzene (method 2) as feedstock. For both pathways, the full process was systematically designed and modeled using Aspen Plus, the required capital costs were estimated by sizing and costing the major process equipment and, combined with the OPEX, a break-even price for NEC was estimated. Additionally, the sustainability and safety of the processes were evaluated. The break-even NEC selling price for both production methods was calculated to be around €2.75/kg LOHC based on a production capacity of 225 ktpa, which is about half the price generally reported in the literature for other LOHC [4]. This significantly improves the economic viability of using NEC as LOHC. The total fixed capital costs were calculated to be around $150MM for both methods of which about 50% are the primary ISBL costs. A major part of the investment costs originates from the reactors, accounting for 63% and 66% of the total for methods 1 and 2, respectively. Additionally, the feedstock contributed to 79% and 77% of the total OPEX of each method. Consequently, the prices of these feedstock show the largest influence on the final break-even NEC selling prices.

References

[1]: P. Preuster, C. Papp, and P. Wasserscheid. Accounts of chemical research, 50(1): 74–85, 2017. doi: 10.1021/ACS.ACCOUNTS.6B00474.

[2]: A. Sartbaeva, V.L. Kuznetsov, S.A. Wells, and P.P. Edwards. Energy Environmental Science, 1: 79-85, 2017. doi: 10.1039/B810104N.

[3]: P.M. Modisha, C.N.M. Ouma, R. Garidzirai, P. Wasserscheid, and D. Bessarabov. Energy & Fuels, 33(4): 2778–2796, 2019. doi: 10.1021/acs.energyfuels.9b00296.

[4]: HySTOC. LOHC production”

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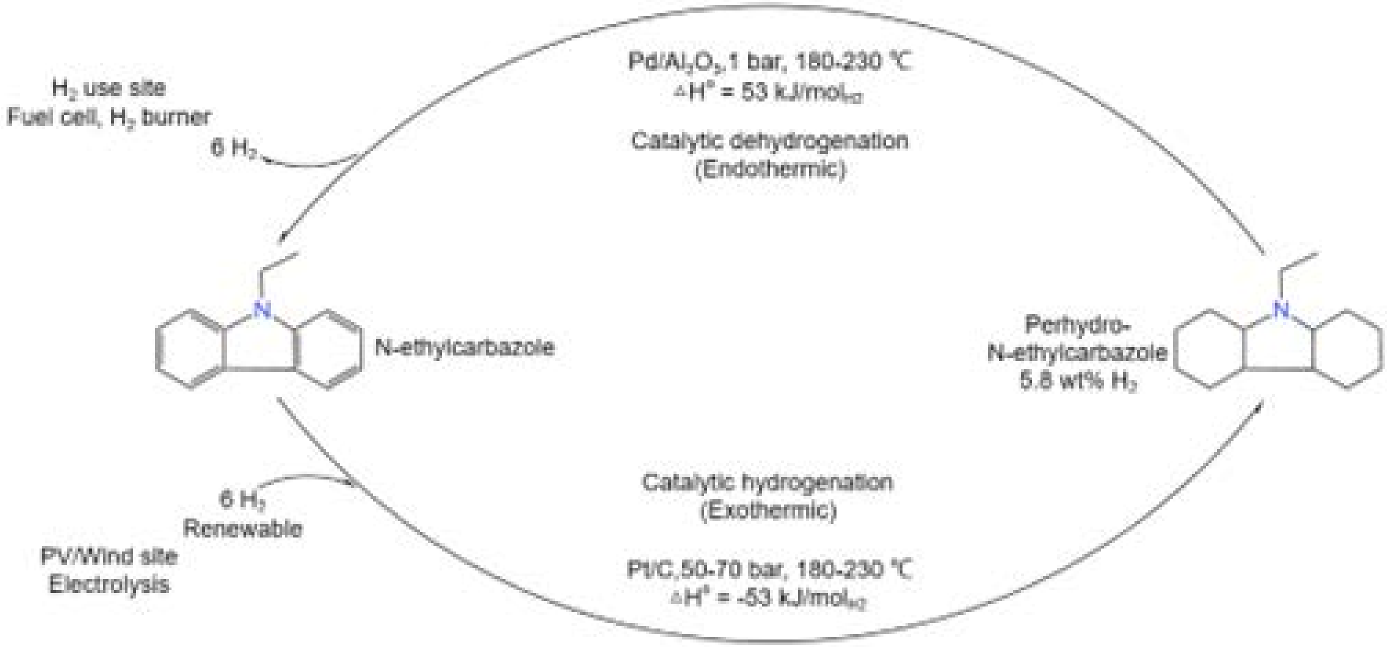

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Title: **[P11] Verification of the Nanoparticle Heating Mechanism in Laser-Induced Nucleation of KCl Solution**

Abstract: Non-photochemical laser-induced nucleation (NPLIN) refers to using short (usually nanosecond) laser pulses to induce crystallization and brings no photochemical damage to the system. Some reports proposed the nanoparticle heating mechanism where heating of nanoparticles in solution under laser causes vapor bubbles and provides nucleation sites near the interface. More work is still required to explore the effect of impurity nanoparticles in NPLIN. We propose two hypotheses to further prove the nanoparticle heating mechanism on the basis of the vapor cavitation model.
1) Increasing the size of the nanoparticles would form larger bubbles and lead to higher nucleation probability;
2) Using nanoparticles with larger absorption efficiency would form larger bubbles and lead to higher nucleation probability.
Different sizes and materials of nanoparticles are added to filtered KCl solution with various supersaturation (1.03 and 1.05) and the nucleation probability will be tested under laser (532 and 1064 nm) to verify these two hypotheses and the nanoparticle heating mechanism.

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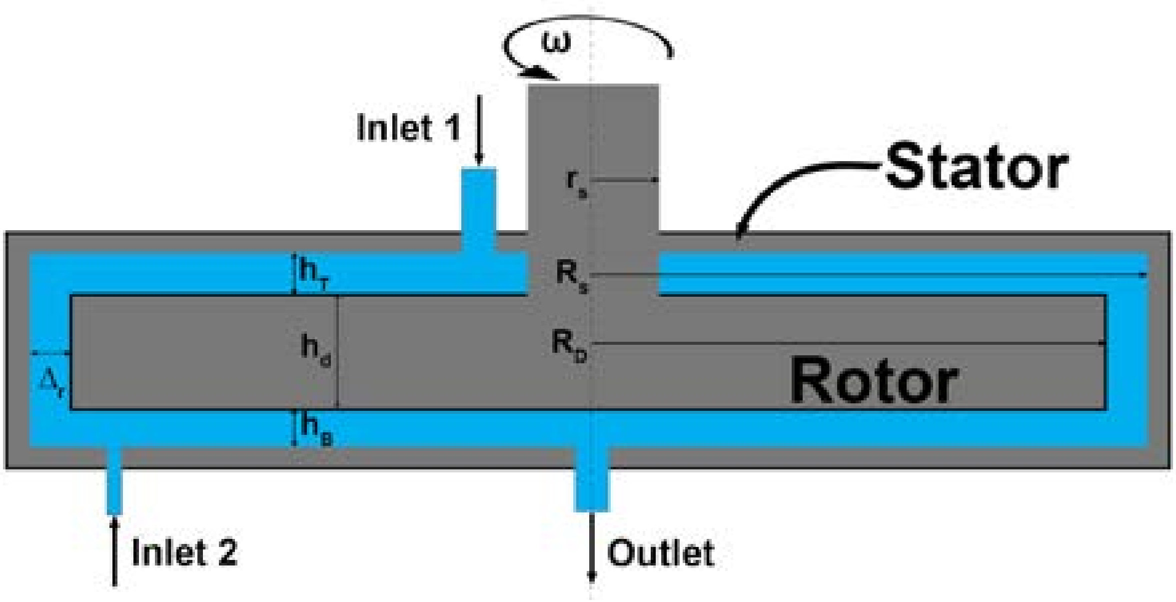
Title: **[P12] Micromixing efficiency in the turbulent boundary layers in a rotor-stator spinning disc reactor**

Abstract: During this work, the Villermaux-Dushman reaction in combination with an injection probe was used to experimentally determine the micromixing times in a rotor-stator Spinning Disc Reactor (rs-SDR), see attached image. The experiments were performed at different axial distances between the rotor and stator and it was found that the mixing intensity was the highest near the rotor (Von Kármán layer) and the lowest near the stator (Bödewadt layer). However, the results deviated from the engulfment model and this was due to the disturbance of the flow field by the injection probe. This was also verified by an analyses in SolidWorks. Besides the experimental investigation, a CFD model with Large Eddy Simulations (LES) in combination with Wall Adapting Local Eddy (WALE) sub-grid-scale model was constructed in OpenFOAM 9. However, the simulated domain only contained the top half of the rs-SDR (single rotor-stator cavity) and the simulation was validated with velocity profiles presented in literature. The validated flow field was used to determine the micromixing times in Matlab and the obtained results were compared with the experimental mixing times. The simulated values were within the experimental error for the inviscid core, but were deviating in the boundary layers. This was due to the difference in dimensionless gap distance, since it reduces the velocity gradient and therefore also the energy dissipation, which is correlated to the micromixing time. The results provided new insights and more knowledge about the optimal micromixing location, namely the Von Kármán layer.



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Title: **[P13] Experimental studies on pressure drop and heat transfer in 3D printed baffled logpile structures**

Abstract: Additive manufacturing, or 3D-printing, of catalyst materials allows structuring of catalytic reactor internals with a degree of design freedom that cannot be achieved through conventional methods of reactor manufacturing. Recent literature has mainly focused on the implementation of so-called “log-pile structures” which consist of stacked cylindrical features. The benefits of this design include, but are not limited to, that it is easier to print with 3D printing methods such as DIW, and, when alternated by 90° for every layer, can fully support itself without external influence. However, in order to be able to provide a meaningful alternative to conventional reactor types such as packed bed reactors, novel 3D-printed structures need to prove their process intensification viability. One method of doing this is to increase the wall-to-bed heat transfer rate, but this, in general, results in increased pressure drop, which would result in increased operation costs. However, 3D printing allows for careful tuning of all design parameters in order to provide the most flexible window of operating conditions. This work shows our experimental efforts to investigate the effect of relevant design parameters on the performance of such 3D-printed logpile catalyst structures. This study functions as an early proof-of-concept of 3D-printed reactor engineering. For this reason, the structures were constructed of PETG rather than catalytically active material, and the focus will primarily be on the pressure drop and heat transfer. A critical optimization variable is the spacing between logs within baffled logpile structures, where a distance of 50 µm between logs in a baffle is shown to decrease the pressure drop over the reactor by 68%, compared to a non-porous baffle. Heat transport characteristics are investigated by monitoring the axial temperature profile of the center and wall of the module at varying flow rates. The effect of relevant design parameters of a 3D-printed logpile reactor on the pressure drop and radial heat transfer will be discussed, including considerations on the viability of implementation of these structures in reactive applications.

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Title: **[P14] Integrating CO2 capture and electrochemical conversion using a bicarbonate flow cell: optimizing Cu/Ag foam electrode configuration for the production of ethylene and ethanol**

Abstract: The electrochemical reduction of bicarbonate into renewable chemicals has been discussed widely as a means to integrate CO2 capture with CO2 reduction. In this way, the energy intense regeneration of the capture solvent can be replaced by an electrochemical cell, which can be powered by renewable electricity. A bipolar membrane is used to liberate the CO2 from the bicarbonate, which is then reduced at the electrode to the reduction products.

In this work, we investigate the use of a tandem Cu/Ag foam electrode in a bicarbonate flow cell for the reduction of CO2 towards multi carbon products. In tandem electrode systems, the Ag electrode generates a surplus of CO which can then be further reduced to multi carbon products on the Cu electrode. By creating a higher CO concentration, the C-C coupling is enhanced and thus faradaic efficiencies (FE) towards multi carbon products can be increased. This has been proven to work well in aqueous systems, but has not yet been investigated in bicarbonate systems. By strategically placing the Ag and Cu electrode foams, we would like to increase the FE towards ethylene and ethanol in the bicarbonate flow cell system. By using an interdigitated flow pattern, we can increase the convective mass transport. We will investigate 3 different Cu/Ag foam electrode configurations to investigate what the optimum configuration is in our system, focusing on forming ethylene and ethanol. The first electrode configuration uses equal amounts of Ag and Cu foam electrodes. The inlet channel will be covered with Ag foam and the outlet channel with a Cu foam. In this way, the CO2 will first react at the Ag electrode to form CO and before leaving the cell, react at the Cu electrode to form multi carbon products. The second configuration covers both inlet and outlet channels with Cu foam and has Ag foam on the land between the channels. The third configurations looks at layering the Ag and Cu foam on top of each other, placing the Ag foam closer to the membrane and Cu foam near the flow channels. By comparing these different configurations we would like to understand better what the optimum ratio between Cu and Ag foam is in a bicarbonate flow cell for the production of ethylene and ethanol.

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Title: **[P15] Gas crossover in advanced zero-gap alkaline water electrolysis**

Abstract: Conventional alkaline water electrolyzers operate with a finite-gap between the cathode and anode. The ohmic resistance induced by this finite-gap results in energy losses. Therefore, the zero-gap assembly is considered an attractive configuration to perform advanced alkaline water electrolysis. However, gas crossover is enhanced in the zero-gap configuration by supersaturated hydrogen concentrations in the vicinity of the electrode. Different transport mechanisms can contribute to gas crossover through the porous separator, namely diffusion, convection and electrolyte mixing. For well-balanced pressures and industrial flow rates, diffusion is the main contributor to gas crossover. Local supersaturation at the diaphragm interface significantly contributes to gas crossover. There is a clear distinction in gas crossover between zero- and finite-gap designs. For the zero-gap assembly, hydrogen crossover rates were found to increase with current density. In contrast, using a finite-gap configuration, gas crossover was significantly reduced and approached equilibrium diffusion rates. Therefore, advanced alkaline electrolysis is possible in zero-gap design, but enhances gas crossover. Gas crossover is mainly driven by diffusive hydrogen transport and supersaturation at the diaphragm interface plays an important role on gas crossover.

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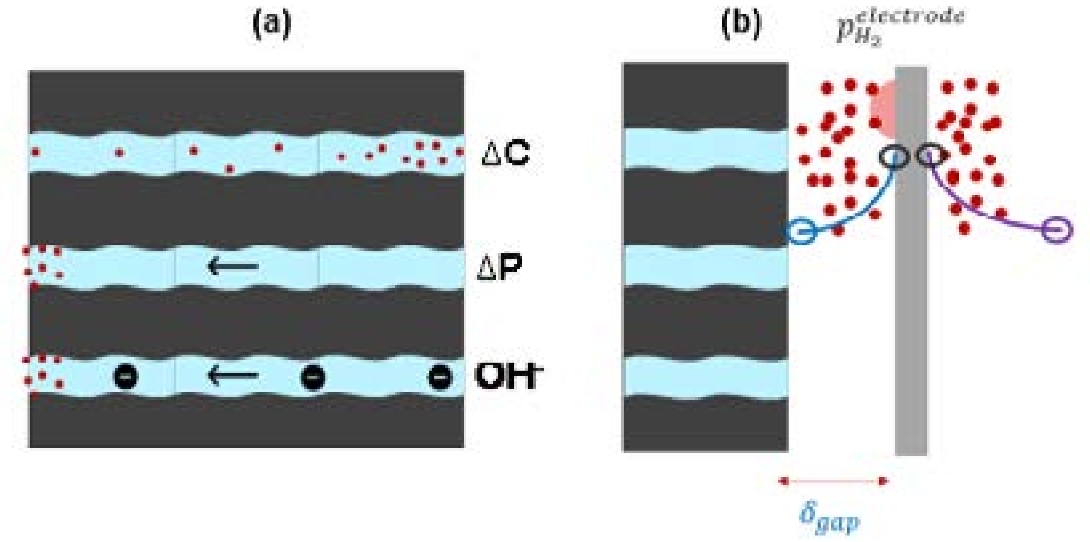

Schematic representations of processes driving gas crossover: (a) diffusion, pressure driven convection and electro-osmotic convection and (b) local supersaturation.

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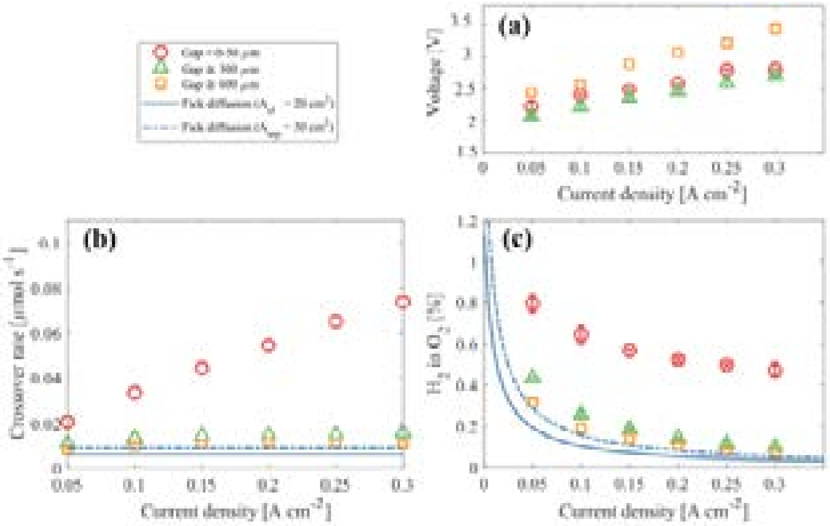

(a) Cell voltage, (b) hydrogen crossover rate and (c) anodic gas impurity as a function of current density at varying gap sizes relative to equilibrium diffusion.
Conditions: 25˚C, 1M KOH, Zirfon UTP220, closed balancing line. Equilibrium diffusion values were calculated using two distinct areas: 1.Electrode area of 20 cm² (straight line) 2.Effective diffusion area 30 cm² (dotted line).

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Title: **[P16] Surrogate models for the optimal design of distillation columns with variable compositions**

Abstract: The rigorous design of distillation columns is essential to provide realistic cost estimations of chemical projects. However, rigorous distillation models are computationally complex (particularly for large sequences) and difficult to integrate with other modelling approaches (e.g. assessment tools or optimization algorithms). Surrogate models have been previously explored to aid in the rigorous design of distillation columns (Quirante et al., 2015; Ibrahim et al., 2015; Bhosekar and Ierapetritou, 2018). However, reliable models that predict the design for variable compositions are still missing. To solve this problem, we propose here a surrogate-based approach for the optimal design of distillation columns to increase the connectivity of rigorous models with a focus on flexible inlet and outlet compositions. The proposed method comprises all the steps required to obtain a fully functional surrogate model, the dataset creation to model fitting and validation. First, we determine the sampling boundaries for the three design variables (i.e. number of trays, reflux ratio, and distillate rate) using short-cut models and use Latin Hypercube sampling to randomly create 10,000 samples. After applying an ordering method to reduce the amount of non-converged samples and avoid unfeasible designs, we use a communication interface implemented in Python to run Aspen HYSYS / Plus for each sample and retrieve the results for products purity and recovery. We then use a filtered dataset to train and validate Artificial Neural Networks (ANNs) to predict the optimal design of a column to achieve a desired product composition. The proposed approach has been validated with a case study on hydrocarbon distillation for monomer recovery from waste plastic pyrolysis (Somoza-Tornos et al., 2020). The surrogate models are correctly fitted and show good accuracies with respect to the rigorous simulation of the column. Future work will extend the approach to other process intensification techniques, such as reactive distillation processes.

References:

Bhosekar, A., Ierapetritou, M. Advances in surrogate based modeling, feasibility analysis, and optimization: A review. Computers & Chemical Engineering 108, 2018, pp. 250-267.

Ibrahim, D., Jobson, M., Li, J., Guillén-Gosálbez, G. Optimization-based design of crude oil distillation units using surrogate column models and a support vector machine. Chemical Engineering Research and Design, 134, 2018, pp. 212-225.

Quirante, N., Javaloyes, J. and Caballero, J.A. Rigorous design of distillation columns using surrogate models based on Kriging interpolation. AIChE Journal, 61, 2015, pp. 2169-2187.

Somoza-Tornos, A., Gonzalez-Garay, A., Pozo, C., Graells, M., Espuña, A. Realizing the potential high benefits of circular economy in the chemical industry: ethylene monomer recovery via polyethylene pyrolysis. ACS Sustainable Chemistry & Engineering 8 (9), 2020, pp. 3561-3572.

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Title: **[P17] Impact of varying macronutrient composition on 3D printability of pea-based food formulations**

Abstract: The emerging technology of 3D food printing is promising for production of personalized foods. Personalized foods are ideal for individual dietary requirements of a consumer, thereby helping to sustain a healthier diet. However, especially changing the macronutrient composition of foods, i.e. the amount of carbohydrates, proteins and fat, is known to strongly affect the printability and buildability of food formulations. In addition, the amount of added water used for preparing formulations plays an important role. The influences of macronutrients and water are complex and have not been studied systematically before. Therefore, the aim of this study was to investigate the influence of macronutrient composition on printability and rheology using a quantitative experimental design approach. For this, a pea-based model food formulation varying in fibre, starch, and protein content was evaluated in terms of printability namely: (a) extrudability and (b) buildability which was further linked with their rheological properties. A systematic study was conducted by varying one macronutrient at a time. Water content was adapted based on water holding capacity of the various ingredients. From the results, it was found that water holding capacity is a good starting point for systematic formulation of printed foods with various macronutrient composition. Subsequently, it was observed that fibre and protein had a stronger effect on extrusion force and flow point than starch, which may be explained by the microstructure of the formulations. Compositions of 30-90% fibre, 10-50% protein, and 0-60% starch on dry basis were identified as the ranges within which stable printed samples could be obtained. The knowledge obtained from this research provides a window of operation for successful 3D printing of pea-based formulations and the approach may be used for other printable food formulations as well.

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Author: Maarten Schutyser (WUR)

Other Authors: Judith Ham, Zulhaj Rizki, Remko Boom (all WUR) and many others from TUE, UT, TUD and RUG

Title: **[P18] Electrically driven non-thermal dewatering of biomass (ELECTRIFIED)**

Abstract:

Drying alone represents around 15-25% of all energy used in the processing industry in the developed world, which is likely to become much more with increasing use of biomass. Sustainable food and biobased processing can only be realized by replacing our current evaporative dewatering processes by processes using more effective driving forces. With a large consortium of universities (WUR, TUE, UT, TUd & RUH) and industrial partners we recently started the NWO KIC project entitled ‘Electrically driven non-thermal dewatering of biomass’ (ELECTRIFIED). In ELECTRIFIED we investigate electric driving forces to extract water from biomaterials, mostly in liquid form. This is done by making use of a combination of molecularly designed electroresponsive hydrogels, well-controlled electro-osmosis and electrohydrodynamic drying. A wide consortium with eight industrial partners ensures the practical relevance of the technologies developed.

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Author: Regina Politiek (WUR)

Other Authors: Julia Keppler, WUR; Marieke Bruins, WUR; Maarten Schutyser, WUR

Title: **[P19] Dry fractionation for sustainable recovery of protein enriched ingredients: A focus on powder properties**

Abstract: Protein ingredients from legumes are of major interest for both research and commercial purposes. Dry fractionation (i.e. milling, and subsequent air classification or electrostatic separation) can be used to produce protein, starch and fibre-rich fractions with a clean label and lower environmental impact than traditional wet fractionation. The native states of protein and starch are preserved upon dry fractionation and allows making of ingredient fractions that exhibit unique functional properties. High relative humidity (RH) upon storage and higher oil contents can negatively influence the milling and dry fractionation behaviour of legumes, which would be related to reduced particle flowability. Our focus is thus to establish optimal dry fractionation of legume flours by unravelling the effect of RH and oil content on powder properties (particle- size, dispersibility and flowability) and process performance (milling, air classification and/or electrostatic separation) (Figure 1). Soybean oil was mechanically removed prior to fine milling to evaluate the effect of oil content on milling performance and particle size and dispersibility. Furthermore, we varied the humidity of the processing air and storage environment between 30% and 70% for milling and air classification of yellow pea (0.8 %DM oil) and chickpea (5.2 %DM oil). We used a pressure titration to evaluate the particle size and dispersibility and we adopted a dynamic measurement sequence based on a descending and ascending movement of a rotating blade to assess the flowability of the produced and stored flours. We found that a higher oil content limits milling to smaller particles and results in less dispersible fine particles below 10 μm (i.e. protein bodies), which might hamper further separation. A change in the RH during milling and air classification does not significantly affect milling- and separation performance in the range of 30-70% RH. However, storage (1 week) of chickpea flour at a humidity of 70% decreased the air classification performance due to a lower particle dispersibility and flowability. Thus, a relative humidity above 70% should be prevented to perform robust air classification. Improving the particle dispersibility and flowability of legume flours by de-oiling or by keeping the RH below 70% improves milling and dry separation of legumes. This enables a more effective use of the biomass with a reduced environmental impact.

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Author: Leyla Ozkan (TU/e)

Other Authors: D.C. Monsalve Sanchez: TU/e, J.H.A. Ludlage:TU/e, C.R. Portilla: TU/e, and M.W.J. Prins TU/e and Helia Biomonitoring

Title: **[P20] Assessment of a bio-molecular sensor in the operation of adsorption processes-A model based approach**

Abstract: Adoption of digitalisation and Industry 4.0 concepts is gaining pace in food manufacturing and bio-based processes [1]. An essential aspect is the introduction of real time sensors in order to improve process monitoring, decision making and process control. To this end, we assess the use of a novel technology for the real-time sensing of biomolecular substances [2, 3] for the monitoring and control of adsorption processes in the food industry.

In recent years, the mechanistic modeling of adsorption processes has got attention since they can be used in optimization, scale-up etc. However, the development of bottom-up models takes a long time and requires estimation of several process parameters from experimental data. Instead, we make use of simple mathematical models (double exponential or logistic function, [4]) to describe adsorption breakthrough curves, which express the concentration of an adsorbate in the fluid phase at the outlet of an adsorption column as a function of time [5]. Our work shows that such a simple model can be used to study how a biosensor placed at the inlet of a column can be used to steer decisions when to stop the adsorptions process. Furthermore, the model can also be used to design a feedback -feedforward control strategy to achieve a constant concentration at the outlet of a series of adsorption columns which was studied for an extraction process of an anti-nutritional factor. The results of our study shows that the integration of a real-time sensing technology could help to track, analyze and optimize production processes in the food industry. This work was partly funded by The Netherlands Topsectors Agri&Food, HTSM, and Chemistry under contract number LWV20.117.

References

[1] D. I. Gerogiorgis and S. Bakalis, Digitalisation of Food and Beverage Manufacturing, Food and Bioproducts, Vol: 128, 2021.

[2] A. Buskermolen et.al., Continuous biomarker monitoring with single molecule resolution by measuring free particle motion, Nature Communications, 13, 1,2022

[3] E. Visser et.al., Continuous biomarker monitoring by particle mobility sensing with single molecule resolution, Nature Communications, 9,1 , 2018

[4] H. Qili, Modifications of Breakthrough Models for fixed Bed Column and Insights into Physcial Meanings of Corresponding Parameters, PhD Thesis, The University of Tsukuba, 2109

[5] A. Pourseedesfahani et.al., Prediction of adsorption isotherms from breakthrough curves, Mi- croporous and Mesoporous Materials, Vol 277,p:237–244 2019

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Author: Hans van de Vorst (SecuoS)

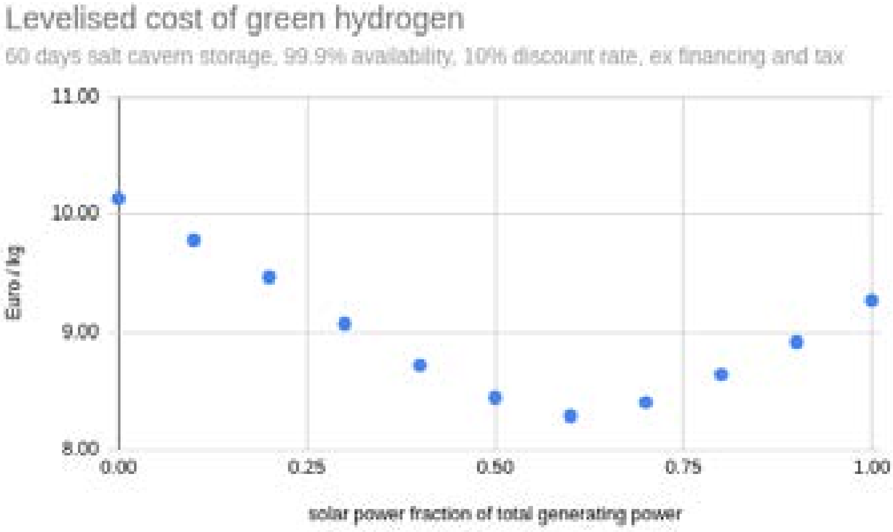
Other Authors:

Title: **[P21] ARTIS**

Abstract:

ARTIS, the Availability and Reliability Tracking Information System, is a web-based application for calculating the available capacity of continuous production and consumption systems. ARTIS has been designed for large and complex systems that consist of many facilities, each of which may be subject to capacity variations, inspection, testing, failure, repair and maintenance. It is applied to renewable energy projects, oil and gas projects, gas liquefaction plants, refineries, chemical plants, power plants and transport networks.

The poster will take the form of a Live demo of the optimisation of an integrated green hydrogen project. Would you be able to arrange a large size monitor and an internet connection?



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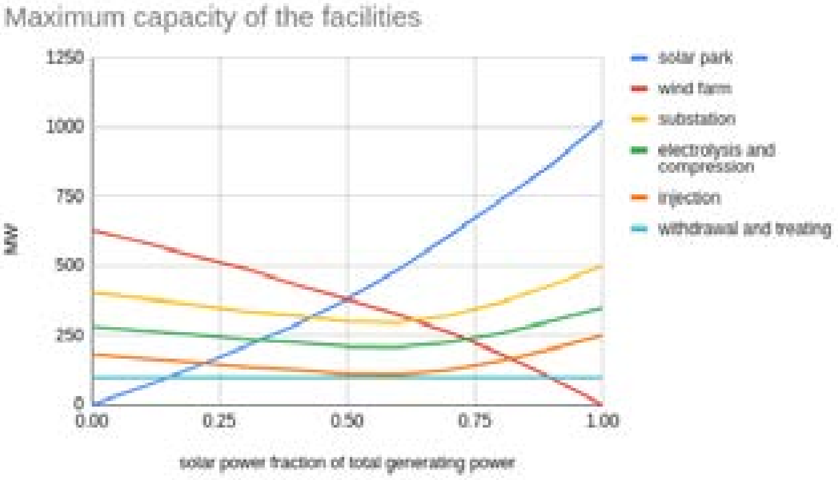

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Other Authors: Z. Li, University of Twente ; N. Kyriakou, University of Twente; A. Nijmeijer, University of Twente; L. Winnubst, University of Twente; MA. Pizzoccaro-Zilamy, University of Twente

Title: **[P22] Tuning mesoporous ceramic membranes for solvent nanofiltration**

Abstract: Membranes, based on ceramic materials, are interesting because of their robustness and can therefore be applied under several demanding conditions, like recovery of valuable products or (organic) solvents. Not only robustness but also pore size and membrane-solvent-solute interactions are important to obtain membranes with the required separation properties. In our work, the surface of mesoporous γ-alumina layers (Øpore ≈ 5 nm) supported on alumina macroporous supports is tuned to prepare hybrid membranes for the nanofiltration of organic solvent solutions [1]. We will present two different types of grafted ceramic membranes. The first hybrid membranes were prepared by grafting small PEG polymer chains using a new synthesis method, showing good performance in solvent-resistant filtration. The new method, developed in our work, involved a pre-impregnation step that plays a pivotal role in initiating weak bond formation between the linking functions and the ceramic membrane before the grafting reaction resulting in the formation of strong bonds and stable hybrid PEG-ceramic membranes. This was confirmed by advanced characterization techniques such as solid-state NMR. The stability of the chemical bonding between precursor and ceramic was tested at room temperature in water and evidenced by water permeation measurements and liquid phase 1H NMR [2]. The influence of the solvent polarity on the conformation of the grafted PEG brush inside the γ-alumina mesopores proved to be key in the analysis of the results and was studied for the first time through molecular dynamic simulations. Finally, the resulting hybrid ceramic membranes showed a very efficient and stable separation of small organic dye molecules such as Rhodamine B (479 g mol-1). Therefore, our membrane material opens up possibilities for a multitude of separations where valuable molecules must be separated from solvents. Secondly, the first preliminary results obtained with the same procedure but using alkyl-based molecules, instead of PEG polymers, will be shown. The influence of the alkyl-chain length was found to be a key in controlling the final membrane pore size. The membranes have been tested for the removal of solutes (< 1000 Da) in apolar and polar organic solvents, and the results will be presented. In conclusion, the inherent chemical and mechanical resistance of ceramics coupled with the multitude of possible grafts can result in three major benefits for grafted ceramic membranes: long membrane lifetimes, suitability to harsh conditions, and the ability to be tailored to a large range of applications.

[1] R.B. Merlet, M.A. Pizzoccaro-Zilamy, A. Nijmeijer, and L. Winnubst, “Hybrid ceramic membranes for organic solvent nanofiltration: State-of-the-art and challenges” J. Memb. Sci. 599, 117839 (2022).

[2] N. Kyriakou, M.A. Pizzoccaro-Zilamy, A. Nijmeijer, M. Luiten-Olieman, and L. Winnubst, “Hydrolytic stability of PEG-grafted γ-alumina membranes: Alkoxysilane vs phosphonic acid

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Author: Dhoni Hartanto (TU Delft)

Other Authors: Hilbert Keestrac, University of Twente; Boelo Schuurc, University of Twente: Anton A Kiss, University of Delft: André B. de Haan, University of Delft

Title: **[P23] Selection of green organic entrainers and natural deep eutectic solvents (NADESs) for azeotrope/close-boiling mixture separation by extractive distillation**

Abstract: Green organic entrainers and natural deep eutectic solvents (NADESs) with a high boiling point and a high decomposition temperature can be promising green entrainers for extractive distillation. This study evaluated the selection parameters, investigated the performance and proposed a selection of green organic entrainers and NADESs for the separation of methylcyclohexane-toluene as a close boiling mixture and n-hexane-ethanol as an azeotrope mixture based. This selection was based on the selectivity and relative volatility calculated using COSMO-RS, UNIFAC and UNIFAC Dortmund as predictive models. Unimolecular quantum chemical calculations with COSMO-RS were used to predict the selectivity at infinite dilution. The group contribution methods UNIFAC and UNIFAC Dortmund were used to predict the relative volatility. According to the calculated results, selectivity appeared a more important selection parameter than the performance index. Relative volatility prediction with UNIFAC and UNIFAC Dortmund showed similar trends as the selectivity results obtained from COSMO-RS. However, UNIFAC and UNIFAC Dortmund cannot be used to predict the relative volatility of the mixtures with the addition of NADESs due to the unavailability of functional group parameters. This study revealed that, based on the calculated selectivities and/or relative volatilities, most of the proposed green organic entrainers and NADESs either outperform or perform comparable to currently used benchmark entrainers. This indicates the potential feasibility of green entrainers to replace the benchmark entrainers for the separation of methylcyclohexane-toluene and n-hexane-ethanol by extractive distillation.

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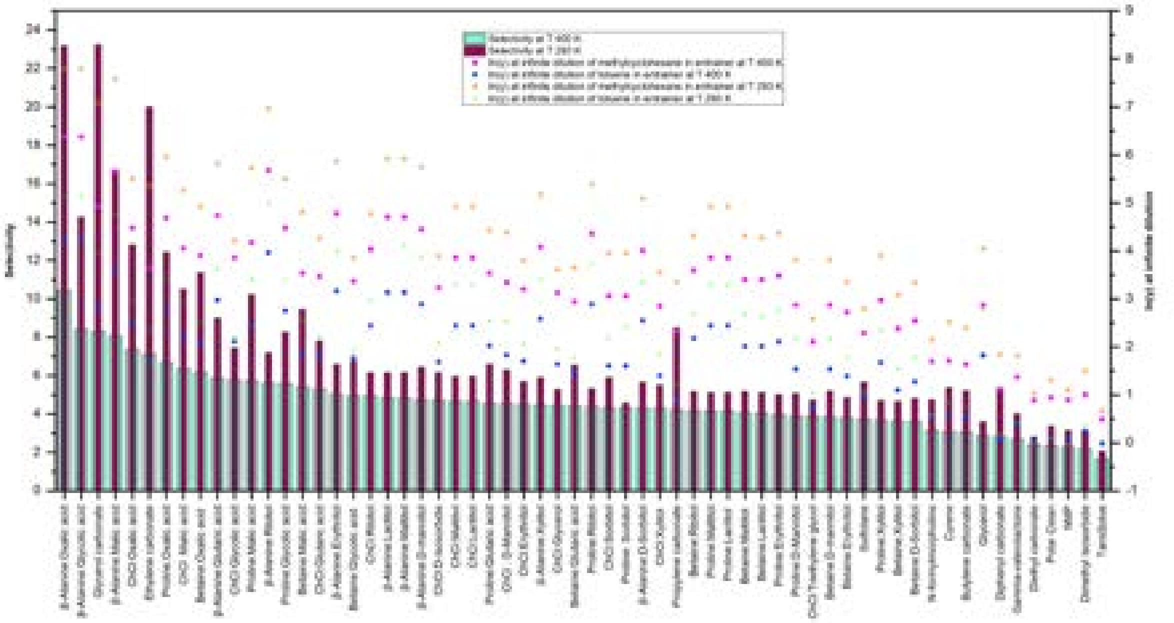

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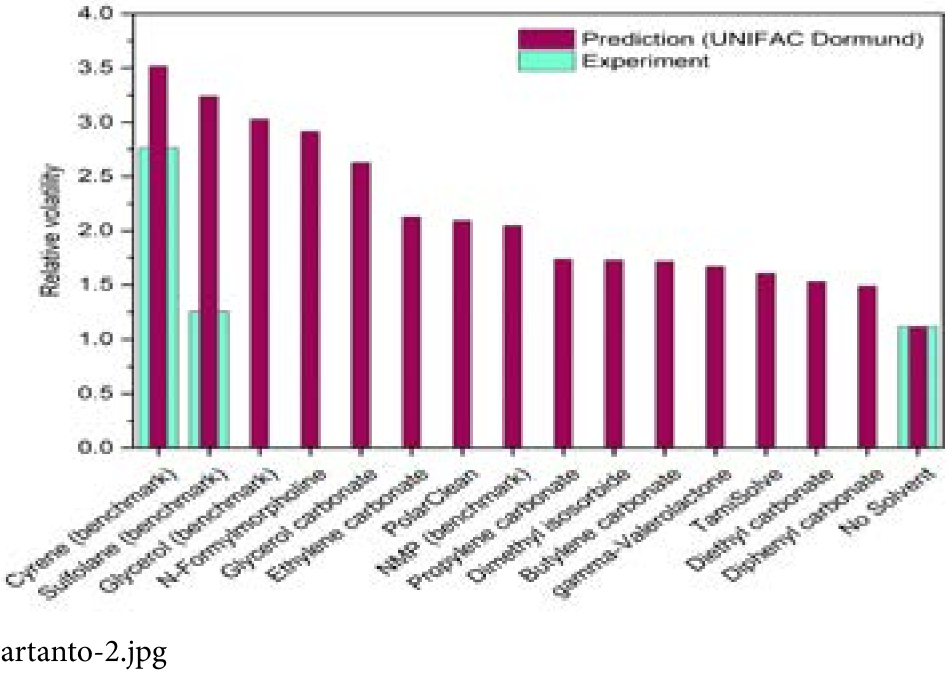

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Author: Weiran Zhang (TU/e)

Other Authors: Ivo Roghair, TU/e; Martin van Sint Annaland, TU/e

Title:

[P24] Study on turbulent flow and droplets behavior to optimize coalescence filter separators

Abstract:

In the screw compressor system, the oil-gas separator is a crucial equipment to separate off lubrication oil droplets via primary separation (separation of the larger droplets with the diameter greater than 5-10μm) and re-separation (separation of the smaller droplets with the diameter less than 5-10μm). To better known the droplets mechanism in the re-separation part is very important for optimizing the whole oil-gas separator. In the part of re-separation, the filter separator is made of fiber materials which has a very complex structure. In this project, we will optimize a simulation approach to investigate the detailed behaviors of microdroplets in the microscope structure, such as microdroplets coalescence behaviors on the single microscope fiber.

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Author: Esli Diepenbroek (UTwente)

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Title: **[P25] Electro-responsive hydrogels for implementation in dewatering and deionizing processes**

Abstract: Biomaterial and food streams typically contain large amounts of water, which challenge the throughput of their transport. To overcome this challenge, removing water from such streams is a common practice. The drying of biomass is currently done by a highly energy intensive evaporation process and takes up a staggering 15-20% of the total energy consumption in developed countries. More energy-efficient alternatives for evaporation would thus have an immense impact on the total energy footprint. Herein, an alternative route with great potential is the development of electrically-driven drying technologies. A promising component for e-driven separation processes is an electro-responsive hydrogel. By using charged monomers to synthesize hydrogels, the water and ion absorption capability can be tuned in and influenced by an electric field. The integration of hydrogels in a drying technology allows for energy-efficient dewatering, as well as circularity of water due to its stimuli-responsive swelling behavior. This poster presents experimental results on the water absorption and structural properties of electro-responsive hydrogels with varying charge densities. The charge density was tuned by using two different types of monomers. Their electro-responsiveness and swelling behavior in pure water and saline water were tested to mimic ion-containing biomass.

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Author: Liang-Shin Wang (TU/e)

Other Authors: Alan Werker, Wetsus; Zandrie Borneman, TU/e; Kitty Nijmeijer, TU/e

Title: **[P26] Properties of polyhydroxyalkanoate membranes formed using non-halogenated solvents**

Abstract:

Though membrane technologies are well-established with ease of use and low energy consumption, the fabrication process needs to be more environmentally friendly and sustainable. Toxic solvents and petrol-based polymeric materials are typically used in the conversion, and this contributes to risks of negative environmental and health impacts. In this research, we use biopolymers from the family of polyhydroxyalkanoates (PHAs) as an alternative for petrol-based polymer membranes.[1] PHAs are fully biobased and biocompatible materials that can contribute to enhancing environmental sustainability and ongoing value in membrane applications. Polyhydroxybutyrate (PHB) and poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) membranes were prepared using evaporation-induced phase separation. So-called PHA-poor non-halogenated solvents, dimethyl carbonate and higher alcohols, were applied as environmentally more sustainable options compared to commonly used chloroform. For PHA-poor solvents, the solubility of PHAs is a function of temperature, concentration, and time. The critical temperatures and times for solvent solutions including solubility and gelation were evaluated systematically by differential scanning calorimetry. The temperature/time criteria were then applied as the key parameters to tailor membrane properties during phase separation. The nature of polymer-solvent interaction and solution concentration were considered and linked to the obtained membrane morphology as well as to the resulting mechanical and thermal properties.

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Author: Peter van der Wal (UTwente)

Other Authors: Sascha R. A. Kersten, University of Twente; Jean-Paul Lange University of Twente, Shell; M. Pilar Ruiz, University of Twente

Title: **[P27] Process development of enhanced furfural production via boronic acid intermediates**

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.[1], [2] 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.[3]
This new method boasts a 95% selectivity, compared to the 50% of traditional methods. To this end, 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. Subsequently, the ester is hydrolyzed to produce furfural at 95% selectivity. So far, this new route has only been done on lab-scale with high-purity chemicals, whereas our work focusses on scaling it up, and adapting it for use with industry-grade reagents. Research activities so far include reducing the amount of boronic acid lost in the extraction step, and checking that the process can handle a real feedstock.

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Author: Martim Chiquetto Policano (UTwente)

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Title: **[P28] Methane oxidation on Pd/CeO2 nanorods, nanocubes and octahedra at low temperatures; structure-dependent activity and poison resistance**

Abstract: A sustainable-driven society combined with restrictive regulations aims to drastically reduce the emissions of health-harmful and global warming gases. In this scenario, the use of liquified natural gas (LNG) vessels instead of the standard heavy fuel oil (HFO) can contribute to reductions in SO2, NOX, CO2, CO, and toxic particles[1]. However, this reduction comes with an increase of around 5 times in methane emissions[1], which is highly undesirable as the methane global warming potential (GWP) is 37±10 in a 100-year lifetime[2]. The strategy to reduce methane emissions is the use of supported noble metals to oxidase methane to CO2[3], which can be captured on-site using liquid and solid adsorbents. Despite the high activity of palladium-based catalysts in dry conditions, the addition of water can deactivate the catalyst by the formation of Pd(OH)2 and hydroxyl accumulation in the support, which consequently hinder oxygen mobility[4]–[6]. Considering that water is generated during methane combustion, the development of water-resistance catalysts is key for large-scale applications. While this inhibition can be reversed by increasing temperature above 450 ºC[7], [8], other deactivation processes are favored at elevated temperatures. At temperatures above 500 ºC, Pd sintering, and support occlusion becomes prominent[6], especially in the presence of water[9]. To overcome this challenge, the adoption of high-mobility oxygen supports, such as CeO2, can increase activity and reduce the impact of water on oxygen availability[6]. Different morphologies of CeO2 can create different facet terminations affecting Pd oxidation state and CeO2 reducibility[10], which can cause changes in the methane oxidation activity. While some articles have addressed this topic[11]–[14], the evaluation of sulfur and water deactivation remains highly unexplored. In this line, this work aims to study the activity and poisoning resistance of different CeO2 facet terminations: nanorods {111}, nanocubes {100}, and octahedrons {110} and {111}, as shown in Figure 1. The CeO2 supports with different morphologies will be synthesized using a hydrothermal method[15] and Pd will be loaded using wet impregnation technique. To underpin the fundamental mechanisms operating in these materials we will combine rigorous reaction kinetics and physicochemical characterization of the different catalysts. This knowledge will be vital in creating structure-property relationships on these materials that can guide the development of industrially relevant methane oxidation catalysts for the maritime industry.

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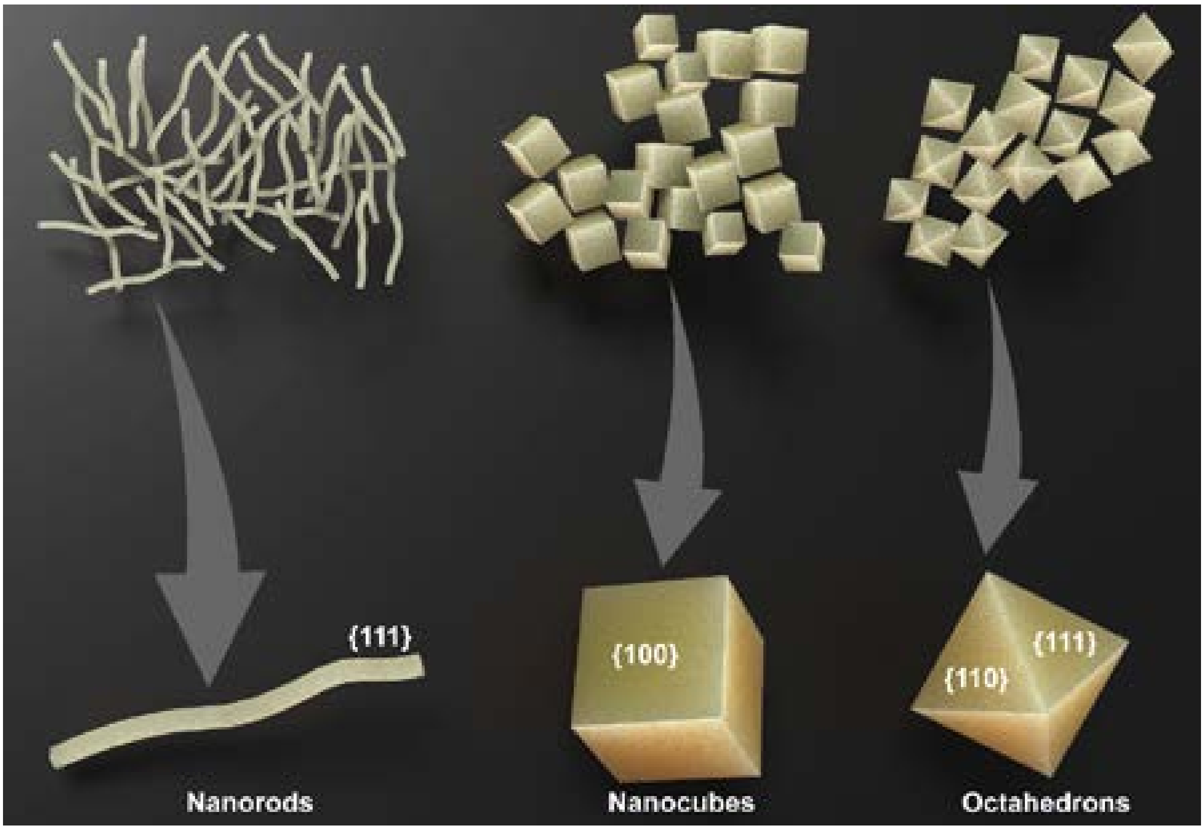

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Title: **[P29] Engineering of two-dimensional nanomaterial layers acting as membranes and reactive electrochemical separation systems**

Abstract: Many industrial processes produce large amounts of aqueous waste streams (10 – 100 m^3/h), contaminated with, e.g. micro/nanoplastics, organic solvents, and/or oxygen-containing molecules. In view of volume and contaminants, the Reactive Electrochemical Membrane technology offers an economically attractive solution for the treatment of these wastewater streams. Reactive Electrochemical Membranes (REM) rely on a combination of physical separation and electrochemical treatment to convert organic contaminants into non-toxic compounds such as water and carbon dioxide. In this system, the wastewater flows through a porous membrane acting as physical barrier and subsequently as active surface (anode) where electrochemically degradation by direct or indirect oxidation occurs. Porous ceramic membranes are widely utilized as support for electrochemical active materials. Sub-stoichiometric titanium oxide-based and B/N-doped reduced graphene oxide-based REM have shown outstanding removal performance but current reported systems are either limited by their small electrochemically active surface areas, large pore sizes or instability. Here we will present our strategy to engineer a high-flux, high-porosity REM with a large electrochemically active surface area, using two-dimensional materials and innovative synthesis approaches.

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Author: Sterre van der Voort (UTwente)

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Title: **[P30] Recyclable Bio-Based Thermoplastic Materials from Liquefied Wood**

Abstract: During a human's lifetime, a person on average in Europe uses more than 100 kg plastic [1]. The largest share of this plastic consumption is fossil fuel based. Therefore, to improve the sustainability of today's plastics industry, fossil commodity plastics can be replaced by bio-based alternatives. However, after more than 20 years of research, these bio-based plastics represent less than one percent of all the plastics produced [2]. They are considered to be uncompetitive compared with fossil commodity plastics due to the usage of expensive feedstocks like edible sugars and the need for comprehensive processing with high purity monomers [3,4]. This work aims to produce a thermoplastic material from cheap and abundant bio-waste feedstock. The lignocellulosic biomass is first converted into a biocrude by liquefaction at 280-320ºC and a pressure of 20-40 bar in the solvent guaiacol within 1-3 hours. The heavy fraction of the liquefaction product, the matrix, can be reinforced with flax fibers (up to 20 wt%). This modification increases the tensile strength of the matrix from 0.4 MPa to 55 MPa [5], which is a value comparable to conventional thermoplastics like polyvinyl chloride and polystyrene. The reinforced thermoplastic can be fully recycled by the same liquefaction procedure as the one performed during the making of the material. Thus, beyond being bio-based, the thermoplastic material is cheap to make and fully recyclable. Further investigation on different alternatives to improve the mechanical properties of the material is currently being developed.

References:

[1] Eurostat, "Packaging waste by waste management operations," ec.europa.eu. https://ec.europa.eu/eurostat/databrowser/view/env_waspac/default/table?lang=en (accessed Jan. 19, 2023).

[2] European Bioplastics, "Bioplastics market development update 2022," 17th European Bioplastics Conference, Dec. 2022, pp. 1-2 [Online]. Available: https://docs.european-bioplastics.org/publications/market_data/2022/Report_Bioplastics_Market_Data_2022_short_version.pdf.

[3] F.C. de Paula, C.B. de Paula, and J. Contiero, "Prospective biodegradable plastics from biomass conversion processes," in Biofuels – state of development, K. Biernat, Ed. London: InTechOpen, 2018, pp. 245-272.

[4] A.K. Mohanty, M. Misra, and L.T. Drzal, "Sustainable bio-composites from renewable resources: opportunities and challenges in the green materials world," Journal of Polymers and the Environment, vol. 10, no. 1, pp. 19-26, 2002, doi: 10.1023/A:1021013921916.

[5] M. P. Ruiz et al., "Fully Recyclable Bio-Based Thermoplastic Materials from Liquefied Wood," ChemSusChem, vol. 12, no. 19, pp. 4395–4399, 2019, doi: 10.1002/CSSC.201901959."

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Author: Aylin Kinik (TU/e)

Other Authors: Kitty Nijmeijer, TU/e; Zandrie Borneman, TU/e

Title:

[P31] Preparation of Electrospun Forward Osmosis Membranes for Clean Water Production

Abstract:

Clean water and clean energy production operations have devoted great attention due to the increasing concern on global warming, water scarcity, and depletion of natural resources [1]. Solar power-based desalination systems are suggested as an alternative sustainable energy production technique to overcome these environmental problems. Recently, researchers have proposed designing an innovative concentrated solar energy (CSP) system including forward osmosis (FO)-based desalination process which recovers the waste heat for producing electricity. The main goal of this system is to create an energy-efficient prototype of the CSP coupled with an FO process to produce desalinated water using both a current and an innovative power cycle while optimizing each constituent of the complete system [2]. FO systems benefit from the naturally generated water diffusion from a low-concentration (feed) solution to a high-concentration (draw) solution through a semi-permeable membrane. However, one of the main challenges in FO is the inefficient membrane supports which cause low water flux and high internal concentration polarization [3]. In order to improve the structural properties of the membrane supports and with that increase the water flux through the membrane, a two-step membrane production method will be investigated. Firstly, mechanically stable highly porous membranes which serve as open support will be prepared via the wire electrospinning technique. In this step, easily hydrolyzed and inexpensive polymers such as polyacrylonitrile (PAN) will be examined. Then, the surface of the membrane will be coated by a layer-by-layer technique with a dense selective layer of a high-performance polymer (e.g. PDADMAC and PSS) based on the electrostatic interaction between the support and the layers. These layers which are stable even at high salt concentrations provide the selectivity not only for water over the draw component but also for water over the NaCl present in the feed solution. Finally, prepared membrane supports will be tested in the FO system for performance analysis.

References

[1] T. S. Chung, X. Li, R. C. Ong, Q. Ge, H. Wang, and G. Han, “Emerging forward osmosis (FO) technologies and challenges ahead for clean water and clean energy applications,”

[2] F. Trieb and D.-I. Hani El Nokraschy, “Concentrating Solar Power for Sea Water Desalination Concentrating Solar Power for Seawater Desalination Concentrating Solar Power for Seawater Desalination,” 2007.

[3] T.-S. Chung, S. Zhang, K. Y. Wang, J. Su, and M. M. Ling, “Forward osmosis processes: Yesterday, today and tomorrow,”

Acknowledgements

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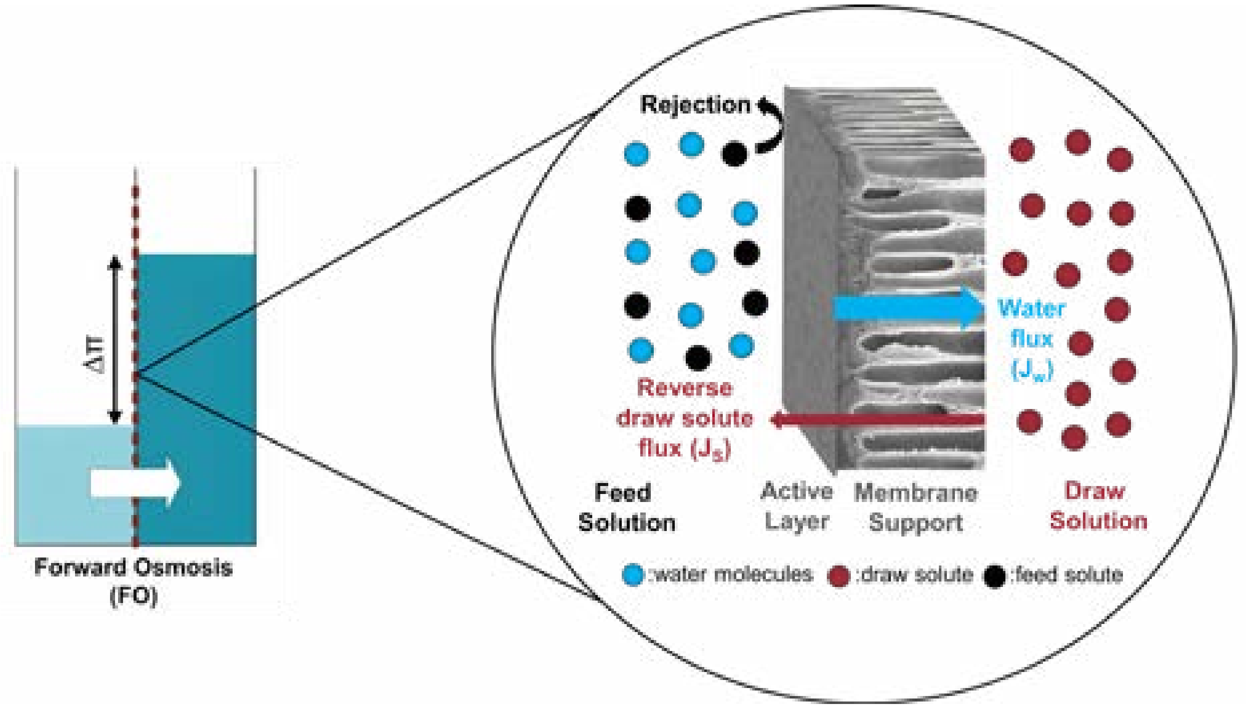

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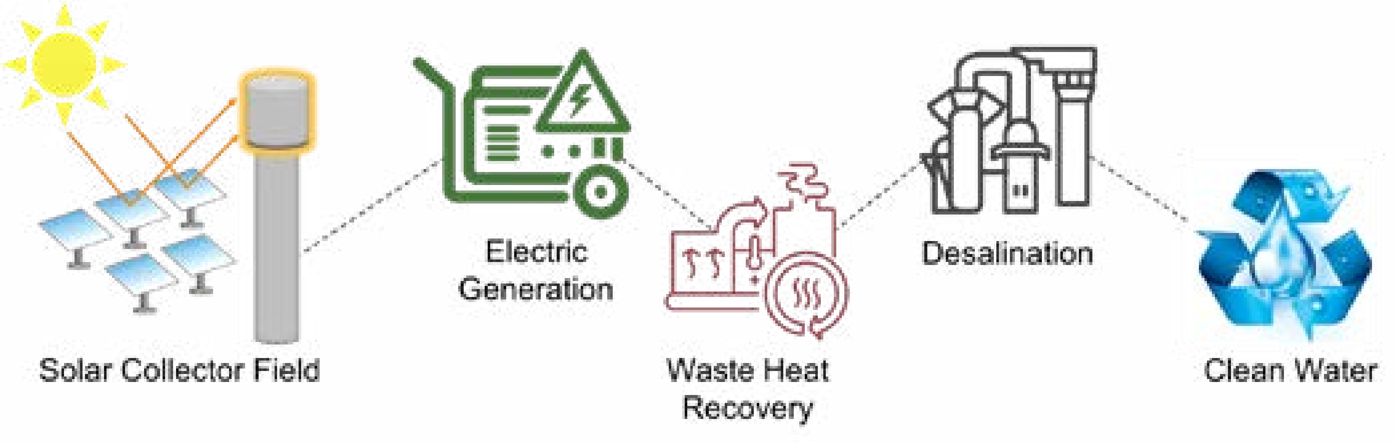

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Title: **[P32] Exploring the detrimental effect of water activity on liquid phase fatty nitrile production for in-situ water removal**

Abstract: To help mitigate the effects of climate change, the chemical industry needs to become more sustainable by using raw materials from renewable resources and by intensifying existing processes. This is also the case for the production of fatty nitriles, which are important chemical intermediates, and can be produced from renewable resources [1]. To produce fatty nitriles, fatty acid and ammonia are reacted as seen in figure 1A. For every mole of nitrile, two moles of water are produced. Removal of water is necessary to increase the nitrile yield and bring the reaction to completion. To intensify nitrilation, a system that combines a reactor with a separation unit is beneficial. There, the water produced during the reaction can be removed in-situ to push the conversion towards completion. To be able to choose the reactor configuration most beneficial for intensifying the nitrilation reaction, the system has to be modeled. For this, the thermodynamic behavior of the gas-liquid interactions has to be known, key for this are the activity coefficients of water and ammonia in the fatty compounds. These activity coefficients are not readily available from literature since their measurement at reaction conditions is complicated by their reaction with the fatty compounds. Therefore, the activity coefficients are simulated to allow a characterization of the system's gas-liquid behavior. The reaction system considered in this work consists of water, ammonia, oleic acid (C18:1), oleic amide and oleic nitrile at typical reaction temperatures of 250-300°C [1] and reaction pressures of 1-8 bar. The activity coefficient of ammonia in oleic nitrile could be measured experimentally since the two compounds do not react with one another. As the other combinations of water and ammonia with oleic acid, oleic amide and oleic nitrile react with each other, their activity coefficients were simulated in COSMO-RS, a quantum chemistry-based thermodynamics model. All molecules were calculated with the GGA:PBE functional and the QZ4P basis set in AMS-ADF. Figure 1B shows the comparison between the experimentally determined activity coefficient of ammonia in oleic nitrile and the simulated activity coefficient of ammonia in nitrile using COSMO-RS. As can be seen, model and experiment are in good agreement in the range of 100-150°C. It also shows that the simulated behavior of ammonia in nitrile at lower temperatures is not ideal and approaches ideal behavior at reaction temperatures. This was also found for the activity coefficients of ammonia in oleic acid and oleic amide.
With the data presented in this work, a comparison between different intensified reactor types such as membrane reactors, reactive distillation, or trickle bed reactors will be carried out. This allows the choice for the intensified reactor type most promising for a more sustainable production of fatty nitriles.

References

[1] A. Mekki-Berrada et.al., ChemSusChem, vol. 6, no. 8, 2013."

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Figure 1A

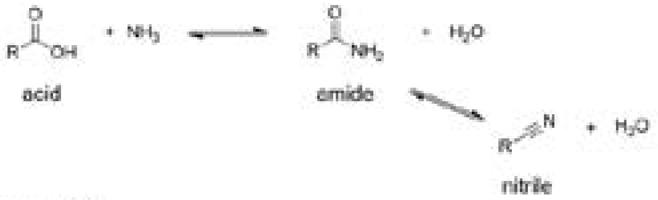
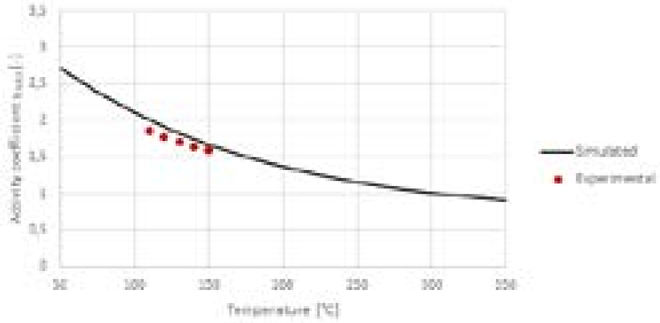


Figure 1B



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Author: Hilbert Keestra (UTwente)

Other Authors: Edwin Zondervan, University of Twente; Wim Brilman, University of Twente

Title: **[P33] The Infinity Reactor: A new conceptual design for a more cost-efficient CO2 to methanol route**

Abstract: Methanol serves as an important building block in the chemical industry. It is a feedstock for about 30% of industrial chemicals 1. Methanol is commercially synthesized from fossil-derived syngas (a mixture of CO, CO2 and H2) via the hydrogenation of CO2, which is an exothermic reaction. The role of CO at high conversions is to remove excess water via the WGS reaction, thereby enhancing CO2 conversions to methanol 2–8. However, this mechanism also increases the exothermicity of the process. Many companies have realised that developing CO2-utilizing technologies may be an essential step towards a more sustainable industrial world 8–13. However, using pure CO2 as a feedstock (e.g. obtained from flue gases to reduce CO2 emissions) reduces the contribution of the WGS reaction and thus increases the water concentration. Catalyst deactivation is one of the major hurdles in green methanol production due to a higher water concentration in the process that induces ZnO agglomeration and ZnAl-spinel formation 14,15. Whereas commercial catalysts have a lifetime of 4-6 years 16–19 with CO-rich syngas-based feeds, methanol production with CO2-rich feeds suffers from rapid deactivation in terms of a few months or even weeks 14,20–22. Therefore, this study has investigated new plant configurations and reactor concepts to improve catalyst lifetime, reduce catalyst usage, and make the CO2 to methanol process more cost-efficient to increase its competitiveness with CO-rich syngas-based methanol production. Boiling water reactors (BWR) and quench reactors are the most utilised reactors in commercial methanol synthesis 23,24 and were therefore used as a starting point for this study. The models of all plant configurations were simulated in Aspen HYSYS and first validated with available plant data from Lurgi 24,25 who utilises a BWR and Johnson Matthey 24,26 (formerly ICI) who uses the quench design. Furthermore, a two-stage reactor concept has been simulated to remove water in-between reactors and it utilises standard unit operations to make the plant configuration easily commercialisable. A shell-and-tube type of reactor with catalyst on both sides is then proposed to allow for heat integration between the reactor endpoints, thus, intensifying the process. Consequently, the average temperature inside the reactors increases and, therefore, the reaction needs less catalyst to reach equilibrium. The quench reactor and adiabatic reactors have been simulated with an operating range of 210-270 °C at 70 bar and the BWR isothermally at 250 °C. This concept saves 35% of catalyst volume compared to adiabatic operation, 20% compared to isothermal operation, and 80% compared to a 4-bed cold-gas injection concept. In addition, the catalyst lifetime is improved due to the lower water partial pressure.

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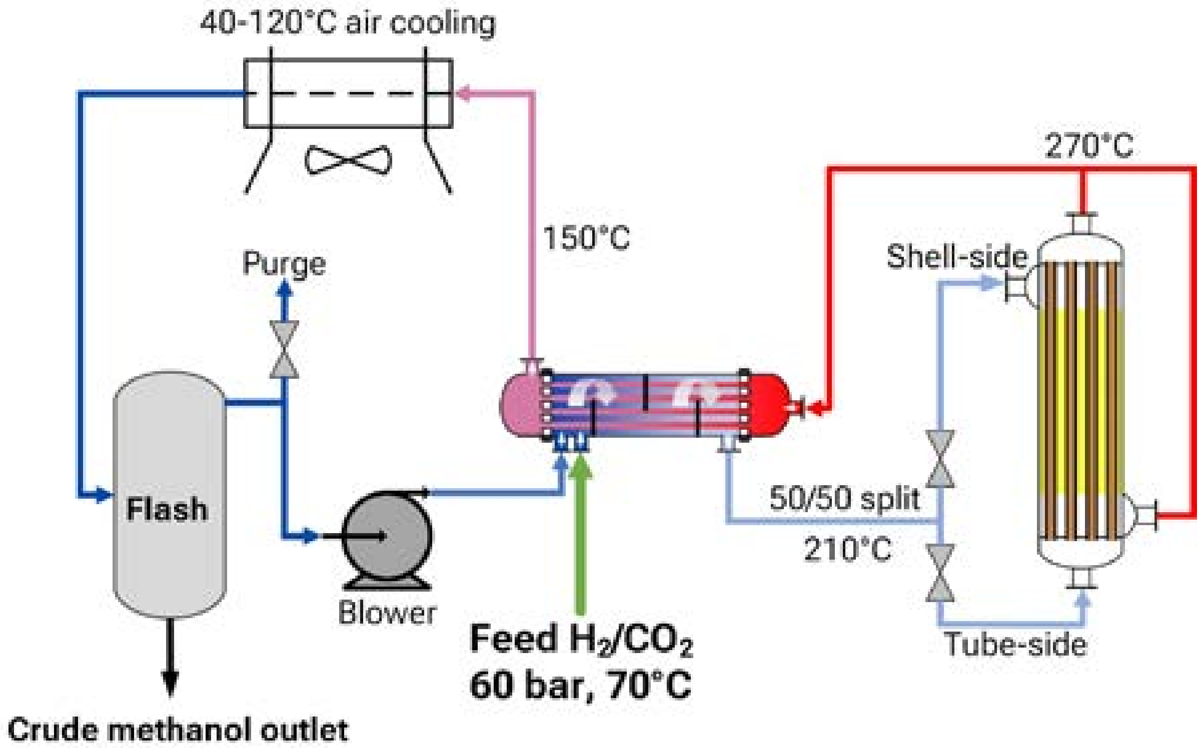

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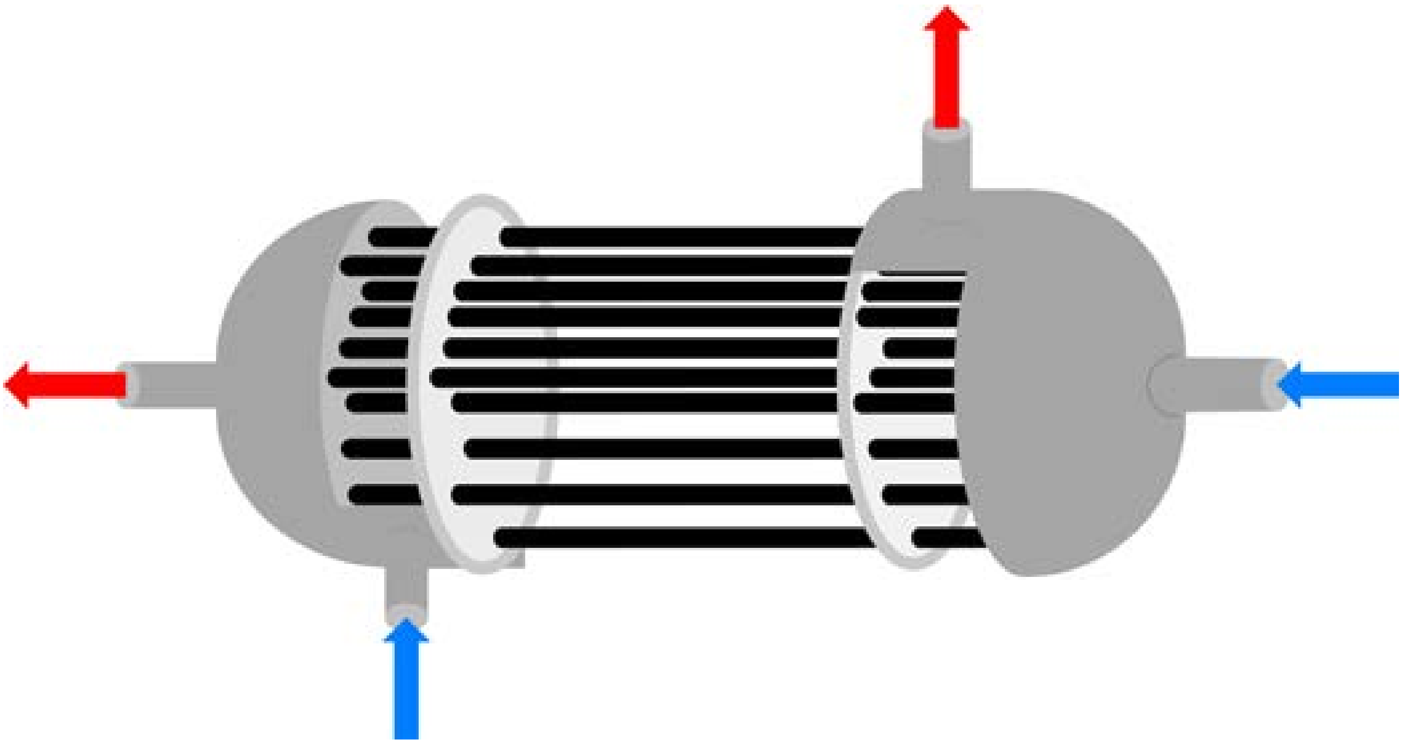

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Author: Soraya Sluijter (TU/e)

Other Authors: G. Elzinga, J. Boon, A. Twerda, S. Sluijter (TNO); L. Wei, I. Roghair en M. van Sint Annaland (TU/e).

Title: **[P34] THOR- Inductive Heating of Processes**

Abstract:

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Author: Liangyuan Wei (TU/e)
Other Authors: Ivo Roghaira, TU/e; Martin van Sint Annaland, TU/e

Title: **[P35] Modeling and simulation of reverse water gas shift reaction with induction heating**

Abstract: A new 3D electrical magnetic field solver was developed for induction heating in OpenFOAM. The temperature dependent electrical conductivity, thermal conductivity and specific heat capacity of magnetic material are included and updated in the solver. Curie temperature of the magnetic material can be set before simulation. The solver was successfully used for 3D induction heating simulations of different coils and magnetic structural materials. The simulation results are consistent with the experimental ones. The bulk magnetic workpiece was heated up from the edge to the center due to the proximity and slot effects. The simulation results showed that a longer coil with many turns is beneficial to obtain a longer uniform magnetic field zone. The experimental results showed that the nano catalyst FeCsCu/Al2O3 can be heated up to 400 in 7 min using induction heating. However, the workpiece should be located as close to the coil as possible for a high induction heating efficiency.

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Author: Riccardo Dal Mas (TU Delft)
Other Authors: Ana Somoza-Tornos, University of Delft; Anton A. Kiss, University of Delft

Title: **[P36] A systems perspective on chemicals manufacturing via electrochemical reduction of CO 2**

Abstract: As the urgency of reducing greenhouse gas emissions increases, the chemical industry is moving towards more sustainable applications, such as substituting fossil feedstocks with renewable ones. The vision of the e-Refinery institute of TU Delft is to promote the development and implementation of novel technologies to allow for the production of chemicals and fuels from CO2 , which will complement bio based productions towards the de fossilisation of the chemical process industry. Given the great importance of the topic, many groups in several institutions around the world are working on the electrochemical reduction of CO 2 (ECO2R) and the large amount of novel developments, paired with the low TRL of these technologies, creates uncertainty in the industry and decision makers. The goal of this contribution is to identify possible routes for the effective conversion of CO2 via ECO2R that are both economically viable and environmentally sustainable, narrowing the focus of the research by eliminating unfeasible options. The great pool of expertise within the e Refinery institute is the starting point for the study, as experimentalists and modelling oriented researchers are working on different areas of the ECO2R ECO2R1 2.The knowledge in these areas can be synthesised into a high level model of a process involving the reduction of CO2 in to one or more chemicals. The following step will be to per from a conceptual process design for a promising conversion route integrated with considerations on the life cycle of raw materials and products and on the coupl ing with a renewable energy system. Challenges in the (electrochemical) reaction separation recycle system will receive particular attention, as they can significantly affect the performance metrics of the process. The study will lead to the identification of some promising CO2 conversion processes, em phasising the representative metrics for their economic and environmental sustainability. The challenges connected to the industrial scale deployment of these novel technologies will be highlighted, with special focus on the requirements for (renewable) electrical energy generation, material usage, and energy intensity of the processes. Conventional production processes will be used as a benchmark for the novel technologies.Preliminary results show that hydrogen and products in which carbon is only partial ly reduced, such as CO, formic acid, methanol, and acetic acid are the most promising, whereas fully reduced hydrocarbons (e.g. methane or ethylene or alcohols (like ethanol or propanol) require very large electric energy inputs undermining their econo mi c ally viable production.

1 Ge, Lei, Hesamoddin Rabiee, Mengran Li, Siddhartha Subramanian, Yao Zheng, Joong Hee Lee, Thomas Burdyny, and Hao Wang. “Electrochemical CO2 Reduction in Membrane Electrode Assemblies.”

2 Sassenburg, Mark, Maria Kelly, Siddhartha Subramanian, Wilson A. Smith, and Thomas Burdyny. “Zero Gap Electrochemical CO 2 Reduction Cells: Challenges and Operational Strategies for Prevention of Salt Precipitation.

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Author: Isabella Arenas Bustos (TU/e)

Other Authors: Xin, Kun, TU/e; Zhou, Qian, TU/e; Sint Annaland, Martin van, TU/e

Title: **[P37] Solvent screening for purification of technical chashew nut shell liquid using COSMO-based methods**

Abstract: In the past decade, there has been a notable trend towards the intelligent utilization of resources. Consequently, the interest in the use of residues and the development of alternative products has increased, in response to the growing global concern for effective waste management. Cashew nut production has been in global growth for the last centuries, but approximately only half of its production represents the kernels (edible nuts), while the other half comprises the residue of the shells, which represents a significant potential due to its valuable composition. Technical CNSL is extracted thermally by roasting the shells and is composed by long chain phenols that include mainly cardol, a dihydric toxic component, and cardanol, that can be polymerized and used for multiple industrial applications, such as dyestuffs, plasticizers, and ion exchange resins. Due to their similar structures and comparable properties, the separation of cardanol and cardol is challenging and subject of research. Different purification methods have been studied and one of the most effective ones is the separation though extraction with solvents. Moreover, COSMO-based methods are novel models fully independent of experimental data that can be used to predict thermophysical properties for liquid systems and have proven to be a valuable tool for predicting vapor pressures, boiling and melting temperatures, densities and VL and LL equilibrium diagrams. This work aims to compare, screen and select promising conventional organic solvents and novel deep eutectic solvents for the purification of technical CNSL to recover a feasible quality and quantity of cardanol through simulations of the extraction with COSMO-based models.

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Author: Romolo Di Sabatino (UTwente)

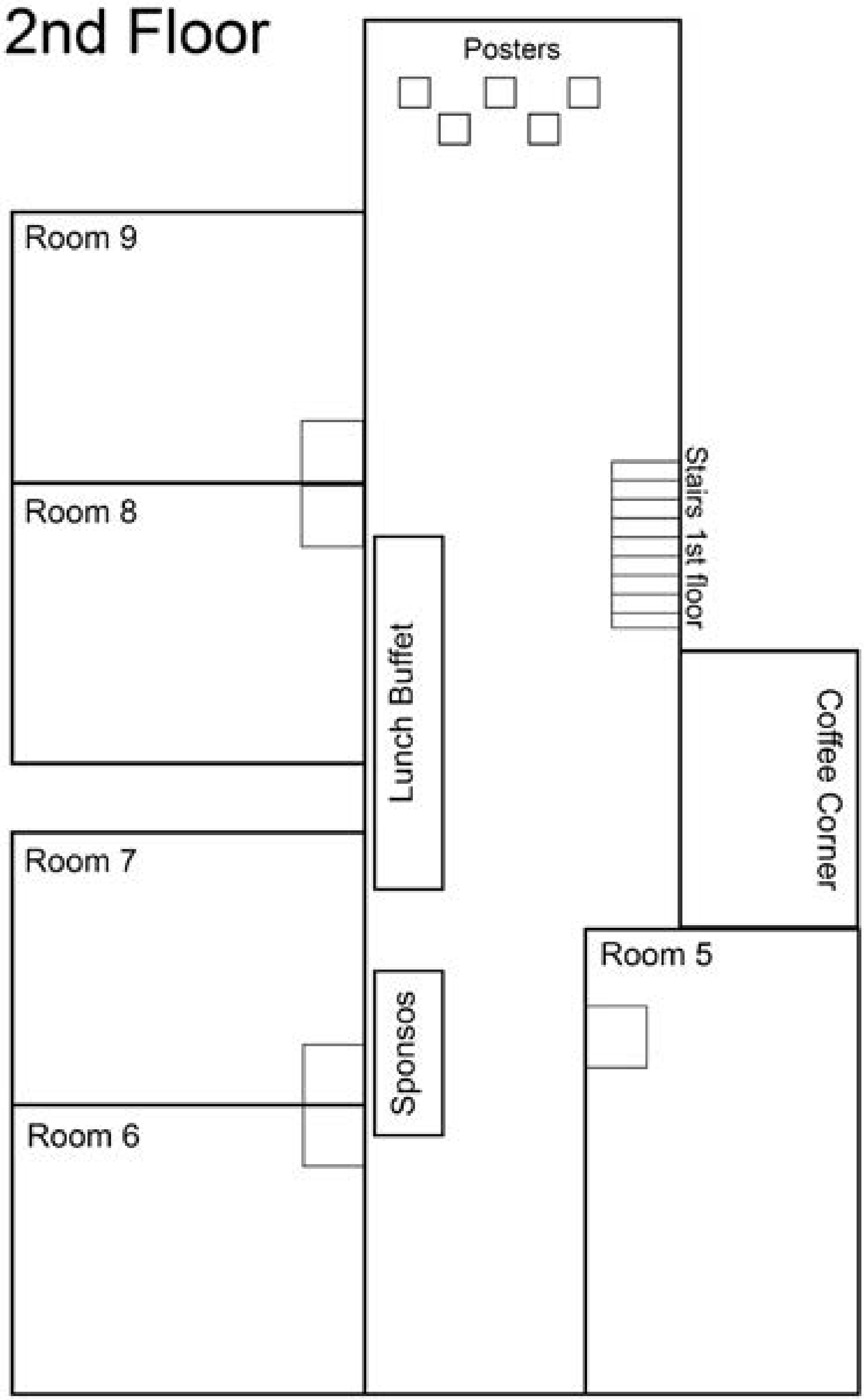
Other Authors: Sascha R. A. Kersten, University of Twente; Jean-Paul Lange, University of Twente; Shell; M. Pilar Ruiz, University of Twente

Title: **[P38] Process development for the conversion of biomass to ethylene glycol**

Abstract: Lignocellulosic biomass is a non-edible and widely available source of saccharides, which can be efficiently converted to ethylene glycol, through catalytic hydrogenolysis over nickel and tungstate catalysts [1][2]. While proceeding efficiently with clean cellulose, the process suffers from low yields when using real lignocellulose. Over the last years, several studies have explored extensive pre-treatments to obtain a clean and saccharide-rich feedstock that can be processed at high yield. It has recently been demonstrated that the main harmful component of lignocellulose is Ca2+, which precipitates the WOx catalyst [2]. Lignin has a less detrimental impact on the reaction that is limited to fouling the Ni hydrogenation catalyst [1]. Based on these learnings, we are exploring an alternative process concept comprising a mild and cheap pre-treatment step and accommodate the burden of remaining contaminants in the downstream process steps. More specifically, we apply minimal pre-treatment avoiding the separation of lignin, and operate the subsequent hydrogenolysis step in the presence of a solvent to minimize detrimental effects caused by the presence of lignin.

This work will report the efficiency of this process, with attention devoted to glycol yield, the nature of lignin, the state of the tungstate catalyst, and chemicals consumption.

Floorplan



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Venue

The conference will be hosted in Kinepolis Enschede, located near the University of Twente campus.

Kinepolis

Colosseum 60
7521 PT Enschede
Netherlands

Directions:

Car - Take exit 26 at Enschede in the direction of Universiteit/Stadion. Follow the road to the left around the 'Grolsch Veste'. You will see Kinepolis Enschede on your right. You can park your car for free in one of the parking lots.

Public Transportation - Take the train to Enschede Kennispark station (formerly Drienerlo). This station can be reached by taking the slow train from Enschede, Hengelo, Zwolle, Deventer or Almelo. Kinepolis Enschede is about a 5 to 10 minute walk from the station.

Wheelchair Accessibility - Kinepolis Enschede is fully accessible to wheelchair users. Elevator and disabled toilets are available.

Accommodation

U Parkhotel, Intercity Hotel Enschede and Fletcher Hotel De Broeierd have a limited number of hotel rooms available for a reduced tariff.

U Parkhotel

De Veldmaat 8
7522 NM Enschede
+31 53 433 1366

Directions:

Car - From the A1 motorway follow the A35 motorway towards Enschede. Than take exit No. 26A Enschede-West/University. At the end of the exit, turn right at the traffic lights and keep following the University signs. Follow the U Parkhotel signs from the University main entrance. On the map of the UT building number 45 (Hogenkamp HO).

Public Transportation (Enschede Kennispark) - Leave the train at stop Enschede Kennispark station. The walking distance from Enschede Kenispark station to the U Parkhotel is approximately 19 minutes.
For the bus: Line 1 towards the University will enter the campus. Leave the bus at stop De Zul. The walking distance from stop De Zul to the U Parkhotel is approximately 3 minutes (300 meters). Line 1 leaves about 4 times per hour and the travel time is approximately 3 minutes.
Lines 8 and 9 to Hengelo do not enter the campus, but stop at the main university entrance (Kennispark/UT). The walking distance to the U Parkhotel is approximately 9 minutes (750 meters).

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(Enschede Central Station) - Leave the train at stop Central Station Enschede.

For the bus: Line 1 towards the University will enter the campus. Leave the bus at stop De Zul. The walking distance from stop De Zul to the U Parkhotel is approximately 3 minutes (300 meters). Line 1 leaves about 4 times per hour and the travel time is approximately 14 minutes.
Lines 8 and 9 to Hengelo do not enter the campus, but stop at the main university entrance (Kennispark / UT). The walking distance from stop Kennispark/UT to the U Parkhotel is approximately 9 minutes (750 meters).

Hengelo Central Station - Lines 8 and 9 run from Hengelo to Enschede will not enter the campus, but stop at the main university entrance (Kennispark/UT). The walking distance from stop Kennispark/UT to the U Parkhotel is approximately 9 minutes (750 meters).

Intercity Hotel Enschede

Willem Wilminkplein 5
7511 PG Enschede
+31 53 20 70000

Directions:

Car - From the A1 motorway follow the A35 motorway towards Enschede. Than take exit No. 26A Enschede-West/University. At the end of the exit, turn right at the traffic lights and keep going straight, following the Centrum signs. At the traffic lights next to Saxion University of Applied Sciences turn left and an immediate right at the next traffic lights. Follow the road until you hit the roundabout and turn right. At the end of the street turn left and an immediate right accros the train tracks. Go around the square and enter the parking garage of Intercity Hotel Enschede.

Public Transportation - Leave the train at stop Enschede Centraal. Go straight when exiting the train station. Keep walking until you the building Metropool. Entrace is near the stairs.

Fletcher Hotel De Broeierd

Hengelosestraat 725
7521 PA Enschede
053 - 850 65 00

Directions:

Car - From the A1 motorway follow the A35 motorway towards Enschede. Than take exit No. 26A Enschede-West/University. At the end of the exit, turn right at the traffic lights and keep following the University signs. After crossing the canal and passing the bridge, turn left at the traffic lights. Take the second road to the right. Hotel De Broeierd will be on your right hand side.

Public Transportation - Leave the train at stop Enschede Kennispark station.

(Enschede Central Station) - Take bus Line 9 to Hengelo CS and exit at stop De Broeierd or take the train to station Enschede Kennispark

(Hengelo Central Station) - ake bus Line 9 to Enschede CS and exit at stop De Broeierd or take the train to station Enschede Kennispark

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Conference Dinner

Brasserie De Bakspieker

Hengelosestraat 725
7521 PA Enschede
053 - 850 65 00

Directions:

Kinepolis - Exit the venue and walk towards the soccer stadium, Grolsch Veste. Go underneath the tracks on the left side of the stadium and keep walking straight until you hit the traffic lights. Turn left before the traffic lights and then De Bakspieker is on your right hand at Fletcher Hotel De Broeierd

*Car - F*rom the A1 motorway follow the A35 motorway towards Enschede. Than take exit No. 26A Enschede-West/University. At the end of the exit, turn right at the traffic lights and keep following the University signs. After crossing the canal and passing the bridge, turn left at the traffic lights. Take the second road to the right. Hotel De Broeierd will be on your right hand side.

Public Transportation - Leave the train at stop Enschede Kennispark station.

(Enschede Central Station) - Take bus Line 9 to Hengelo CS and exit at stop De Broeierd or take the train to station Enschede Kennispark

(Hengelo Central Station) - ake bus Line 9 to Enschede CS and exit at stop De Broeierd or take the train to station Enschede Kennispark

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