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# KEYNOTE Speeches

## Jennifer Holmgren | Becoming CarbonSmart: creating the new carbon economy

The juxtaposition of COVID and Climate is stark: the response to COVID has been swift and bold; the response over the years to Climate Change has been slow, hesitant, and incremental. The world is clearly in crisis mode for COVID – racing to find a vaccine and pursuing all possible approaches, because the world can't afford to develop vaccines at anything but the most rapid pace possible. We must likewise treat Climate Change as the true crisis it is and accelerate the implementation of all new approaches to support our war on carbon.

We must treat deployment of new fuels to address climate change in the same way as COVID vaccines – pursuing all possible technology solutions with an eye to the future. Innovation and Industrial biotechnology hold the key, with a variety of new approaches being commercialized to reduce carbon and produce the things we use in our daily lives.

We currently recycle metals, plastics and paper - so why not recycle carbon?
There is an abundance of carbon locked in wastes from agriculture, forest, unsorted, unrecyclable municipal wastes and in gaseous byproducts of certain manufacturing processes. Biotechnology enables us to convert carbon pollution into everyday products, turning our carbon problem into an economic opportunity keeping the skies and oceans clean and blue for all!

LanzaTech is one such example and has developed a gas fermentation technology that recycles carbon rich industrial off gases from many industries into fuels and chemicals. This technology is operating at commercial scale and represents a novel biological pathway for low carbon fuel and chemical production, while adding value to industrial waste streams. This approach embodies the circular economy taking waste streams to make new products with reduced environmental impact. This presentation will address the scaling up of carbon recycling technology for the production of sustainable, low-cost fuels, chemical-building blocks, materials and food.

## Barbara Mounier | Use Water Twice

Over the last few years, climate change is causing severe droughts. The hydrologic cycle provides insufficient supply for global demand. Water stress is an emerging challenge in many countries all over the world. In the next 30 years, the global population is expected to grow by 2 billion people, with 60% forecasted to live in urban areas, and we will need 55% more water in 2050 than we are using right now. Without changing behaviour, future generations will have insufficient water supply for any acceptable comfort of living in these areas. Yet all around the world, water is still considered to be a cheap resource and people think wastewater is disposable. This must change right now. It's possible to prevent our most valuable resource from being lost by implementing circular water management solutions today.

Decentral water recycling is scientifically recognized as an easy, efficient, and affordable way of utilizing a water source that is already available in the building. By equipping new buildings and retrofitting existing buildings with a decentralized water recycling system, it is possible to collect, treat and reuse slightly used water in the building and give it a second 'loop'.
Hydraloop collects water from bath and shower, washing machine and dryer as well as condensation water from heat pumps and air conditioners. Hydraloop's sustainable technology treats the greywater in six cleaning steps, resulting in clean, clear, safe, and disinfected water for non-potable use. The treated water is redistributed to toilets, washing machines, and optionally for garden irrigation and/or topping up swimming pools.
Hydraloop combines six technologies: sedimentation, floatation, dissolved air floatation, foam fractionation, an aerobic bioreactor, and disinfection with UV light. The decentralized water recycling technology is certified by NSF/ANSI according to the NSF-350 standard, PIA (Germany) and KIWA. The water quality also complies with the European Grey Water Standard and the Australian NSW health standard.

After winning several international awards in 2020, Hydraloop grew from a promising start-up to scale up with global recognition within two years. The company now holds offices in the Netherlands, the United States and the Middle East and works with a rapidly expanding partner network of dealers and installers all over the world, offering different products aimed at residential and commercial real estate. Working closely with local and national stakeholders, such as water utilities, municipalities, and legislators, Hydraloop's vision is that within 10 years, every new build will be built 'Recycle Ready'. For this to become reality, regulations and building codes need to become more focused on water sustainability.

## Kitty Nijmeijer | Together more sustainable: Where chemistry meets technology

With the transition to a sustainable, circular economy and a strong emphasis on the recovery and reuse of materials, minerals and nutrients, separation technology will become increasingly important. Associated to this, the complexity of separations will increase. This requires separation technologies with molecular specificity. Membrane technology is a very versatile separation technology: both membrane characteristics as well as membrane operating parameters determine the ultimate membrane process performance and can thus be used to tailor separation performances towards specific applications.

In line with the theme of NPS 17, ‘Together more sustainable’, this presentation discusses how chemistry and technology together determine the ultimate membrane separation performance. Different membrane preparation methods, both those currently industrially applied as well as more sophisticated methods, will be presented to show how membrane characteristics can be tailored. This will be combined with the effect of operating parameters on the actual membrane process performance in industrially relevant separations.

## Kim Ragaert | Moving beyond the status quo in plastics recycling?

Plastics recycling is a very hot topic, with ambitious European targets closing in rapidly. Have any significant advances really been made in the past decade? Is mechanical recycling really ‘done’ and is chemical recycling really a silver bullet? Where does polymer science feature in all this – if at all?

In the first part of this keynote, prof. Ragaert will address the current state of affairs for plastics recycling in Europe and share some concepts for a way forward. In the second part, she will talk about ‘quality’ in recycled plastics and how we could not only objectively quantify this, but also integrate it in LCA.

# Oral Presentations | Parallel sessions

## THEME: Bioprocess, Food and Pharma

### Eral | Shaping industrial processes with soft matter, light and flow

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| Theme | **Bioprocess, food and pharma** |
| Authors | Burak Eral |
| Affiliation | Delft University of Technology |

With the societal push towards more efficient industrial processes with lower energy and carbon imprint, process engineers are forced to re-think industrial processes. In this talk, I will explore how industrial separation processes can be intensified leveraging soft materials, light and flow. To illustrate my point, I will focus on three examples: (i) Separating micron size particles based on their shape using solely hydrodynamic interactions, (ii) Light induced crystallization of industrial salts and active pharmaceutical ingredients, (iii) Engineering of soft materials to selectively crystallize desired polymorphic form in industrial crystallization.

I will first briefly discuss how particles of all shapes and sizes flowing through tight spaces can be separated based on shape using currently underexplored, omnipresent fluid–structure interactions independent of external intervention. By leveraging experiments, theory, and simulations, we show how the symmetry of a particle determines its overall trajectory: In particular, mirror-symmetric particles, both strongly and weakly confined, follow a universal path. We propose minimalistic scaling relations to describe how particle shape affects the parameterization of the universal path. These findings could be used to “program” particle trajectories in lab-on-a-chip devices and industrial separation processes. Secondly, I will present a combined modelling and experimental study to shed light on how an intense focused light can trigger crystallization in supersaturated solutions, a much-debated phenomena in industrial crystallization. Finally, I will present an experimental study illustrating how surfactants at liquid-liquid interfaces trigger nucleation of a desired polymorphic form through an interplay of surfactant-solute interactions and lattice-matching effects.

# Hop | A study on the effect of shear on Clostridium autoethanogenum in a rotor-stator spinning disc reactor

Theme **Bioprocess, food and pharma**
Authors C.J.W. Hop, M. Benschop, J van der Schaaf
Affiliation Eindhoven University of Technology

Currently researchers are seeking a solution to decrease the global warming effect. This effect is mainly caused by the emission of waste gasses such as carbon dioxide ($CO_2$), carbon monoxide (CO), hydrogen ($H_2$) and nitrogen containing gasses ($NO_x$). A promising and potential solution is gas fermentation by microorganisms (mainly Clostridia species). Clostridium autoethanogenum, an anaerobic bacteria, is used in this project to convert CO gas to renewable fuels and chemicals such as acetic acid, ethanol and 2,3-butanediol. However, the current reactor configurations (stirred tank reactors and bubble columns) require a high volume and there is a limitation in gas-liquid mass transfer. A suitable reactor might be, the rotor-stator spinning disc reactor (RS-SDR). This reactor can increase the gas-liquid mass transfer rate up to 40 times compared to conventional reactors. However, this reactor has not yet been tested and used in a biotechnological process. The large shear forces and high turbulence intensity that arise in the reactor can have a potential negative influence on the bacteria and product formation.

During this study experiments are done in a fed batch and RS-SDR reactor. Data on the gas consumption, bacteria concentration and product formed was gathered over time in both the fed-batch and RS-SDR reactors and compared to each other. Furthermore, image analysis was applied on microscope pictures taken to check for possible changes in bacteria length and shape.

# Puiman | Relieving the mass transfer limitations in syngas-to-ethanol fermentation processes

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|---|---|
| Theme | **Bioprocess, food and pharma** |
| Authors | Lars Puiman, Marina Perdigão Elisiario, A.J.J. Straathof, C. Haringa, H.J. Noorman, C. Picioreanu |
| Affiliation | Delft University of Technology |

Syngas fermentation is a promising process for sustainable production of biofuels and biofuels. The poor solubility of syngas constituents (CO, $H_2$) is often attributed as the major cause for mass transfer limitations in this process (Asimakopoulos et al., 2018; Klasson et al., 1991).

Despite these assumed mass transfer limitations, the company LanzaTech recently succeeded to commercialize a syngas fermentation process (Köpke and Simpson, 2020): By operating a large-sale external-loop gas-lift reactor (EL-GLR), CO-rich steel-mill off-gases are converted into ethanol. High mass transfer rates of about 7-8.5 g.L-1.h-1 have been reported for the industrial-scale process. However, when applying established mass transfer correlations from scientific literature (Garcia-Ochoa and Gomez, 2009) a much poorer performance (0.3-2.7 g.L-1.h-1) is predicted.

We used computational fluid dynamics (CFD) to provide detailed insights on hydrodynamics and mass transfer in a large-scale EL-GLR. As ethanol could increase the gas hold-up (+ 30%) and decrease the bubble diameter (< 2 mm) compared to air-water mixtures, we found with our model that a high volumetric mass transfer coefficient kLa (650-750 h-1) and mass transfer capacity MTC (7.5-8 g.L-1.h-1) for CO are feasible.

Experiments in lab-scale bubble columns confirmed that the presence of ethanol increased the kLa significantly in both water and fermentation broths (2 to 4 times compared to demineralized water). Bubble size analyses show that in all cases very small bubbles are obtained due to the presence of ethanol (0.8 mm). Although we do not know if the bubbles could become that small in large-scale reactors, the CFD model shows that even with 2 mm bubbles the mass transfer limitations can be significantly relieved in gas-to-ethanol fermentation processes.

References

Asimakopoulos, K., Gavala, H.N., Skiadas, I. V., 2018. Reactor systems for syngas fermentation processes: A review. Chem. Eng. J. 348, 732–744. https://doi.org/10.1016/j.cej.2018.05.003

Garcia-Ochoa, F., Gomez, E., 2009. Bioreactor scale-up and oxygen transfer rate in microbial processes: An overview. Biotechnol. Adv. 27, 153–176. https://doi.org/10.1016/j.biotechadv.2008.10.006

Klasson, K.T., Ackerson, M.D., Clausen, E.C., Gaddy, J.L., 1991. Bioreactor design for synthesis gas fermentations. Fuel 70, 605–614. https://doi.org/10.1016/0016-2361(91)90174-9

Köpke, M., Simpson, S.D., 2020. Pollution to products: recycling of 'above ground' carbon by gas fermentation. Curr. Opin. Biotechnol. 65, 180–189. https://doi.org/10.1016/j.copbio.2020.02.017

# Ramirez Calderon | Design of a circularity-based process for bioethanol production using the Delft Design Map

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| Theme | **Bioprocess, food and pharma** |
| Authors | Olga Alejandra Ramirez Calderon, Henrique Maria Cardoso de Menezes de Avelar, Adham Assadbeigi, Pieter L.J. Swinkels |
| Affiliation | Delft University of Technology |

Biobased chemicals and biofuels are key components in the race towards sustainability and circularity. In this category, bioethanol (BE) stands out as a promising alternative to replace fossil fuel-based chemicals with a competitive advantage from perception and regulations perspectives. This project aimed at designing an ingenious large-scale second-generation BE plant applying the Delft Design Map to synthesize creative ideas that could lead to feasible design options. The considered feedstock was switchgrass grown on marginal land.

Based on market analysis and the possibility for synergistic integration with a bio-butadiene (BD) plant, two product concepts were constructed: (1) BE for BD production and (2) BE for biofuels. The design capacity consisted in 320 kton.year-1 for BD and 126 kton.year-1 for biofuels. Pre-treatment with liquid hot water (200 °C) was found to be optimal. For microbial conversion, a co-culture of C. thermocellum and T. saccharolyticum was selected, to achieve hydrolytic, C5, and C6 sugars conversions in a single tank. Decoupling the hydraulic and solids retention times was identified as a crucial task to achieve a sound economic performance. To do this a design option of continuous upflow operation and fluidized bed (dilution rate of 0.5 h-1) was selected.

Process tasks and operational units for lignin valorization through energy recovery were included to improve the economics of the process. It makes the plant self-energy sustainable. Based on a concept feasibility evaluation, the design choices and plant integration lead to good economic potential. Moreover, it shows a $CO_2$ equivalent emission reduction of 112% compared to its fossil fuel counterpart according to the Renewable Energy Directive RED II methodology.

# THEME: Circularity

## Bhatraju | Design of Fossil-Free Butadiene Production using Delft Design Map™

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| Theme | **Circularity** |
| Authors | Bhatraju, C.; de Hoop, D.; Sultan, H.; Swinkels, P.L.J. |
| Affiliation | Delft University of Technology |

1,3 butadiene is a major building block in producing synthetic rubbers used in tyre production. Currently, butadiene is produced in a steam cracker which suffers from low and variable yields, leading to supply instabilities and price volatility. An on-purpose production route is needed and an interesting is the production of butadiene from ethanol. In this project, a process for bio-butadiene production is designed using the Delft Design Map™ and integrated with a bio-ethanol plant. The Delft Design Map™ (DDM) is a 12 step design methodology to design a novel process effectively and efficiently. Using DDM, an innovative process is designed that can produce 145 kta of butadiene.

The designed process has targeted production of butadiene with an yield of 45 wt%, instead of 5wt% of the conventional route, along with seven technical-grade products that can be readily sold in the market. The production process converts ethanol to butadiene in a one-step process, instead of the traditional two-step process, reducing process complexity. The designed process use carbon-neutral raw materials and utilities which reduces the direct $CO_2$ emissions to zero. The economics and sustainability of the process is improved by taking advantage of the synergistic opportunities between the bio-ethanol and bio-butadiene plants. The mutually beneficial relationship with bioethanol producers resulted in a green premium of 10-20%, competitive to other butadiene from ethanol processes while avoiding 100% of fossil fuels in the production process. The green premium can be further reduced to zero through cost optimisation of raw materials and products.

## Dafnomilis | $CO_2$ activation through sorbent enhanced reverse watergas shift

Theme **Circularity**
Authors Antonios Dafnomilis, Francesco Franco, Jenkins Jose Shirley, Namrata Shah
Affiliation Delft University of Technology

To promote the energy transition, a conceptual design is made to assess the potential of the Reverse Water Gas Shift Reaction (RWGS) and to foster its application in 2030. By using $CO_2$ and $H_2$ this reaction produces CO and $H_2O$. CO mixed with $H_2$ is regarded as syngas. When using green $H_2$ and $CO_2$ captured from flue gas or air, the RWGS becomes a sustainable production alternative to fossil fuel syngas.

The thermodynamics show that the endothermic RWGS reaction has negligible conversions below 400°C. In-situ removal of the water product via a sorbent enhanced reactor is used at high $H_2$:$CO_2$ feed ratio to shift the equilibrium allowing for low temperature operation. A fluidised bed reactor is selected since it allows continuous selective regeneration of the sorbent. The sorbent regeneration is done by selectively heating water with microwave, thus drastically reducing (~90%) the duty requirements. Zeolite 3A is selected as sorbent since it can selectively adsorb water due to pore size exclusion. Unconverted $CO_2$ is removed from the syngas by absorption with Selexol and recycled to the reactor.

The plant produces 100 kta of syngas with $H_2$:CO composition of 2:1(Moles). The process reaches 97% $CO_2$ overall conversion. Green $H_2$ accounts for 60% of the OPEX. Currently the production costs of the produced syngas are higher than the price of fossil fuel syngas which makes the process uneconomical. Lower green $H_2$ costs and a green premium for the sustainable syngas price are required for the process to become economically competitive.

## Heijstra | Capturing Carbon, creating value via Gas Fermentation

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| Theme | **Circularity** |
| Authors | Bjorn Heijstra |
| Affiliation | Lanzatech |

The production of biofuels and platform chemicals via gas fermentation is a rapidly developing technology for high volume, sustainable, production of fuels and chemicals that does not require food-based substrates as a feedstock. LanzaTech was founded in 2005 in New Zealand and headquartered on the Northside of Chicago with global offices and facilities.

Over the last 15 years LanzaTech developed and scaled a complete process platform to allow the continuous biological production of fuels and an array of chemical intermediates from gases. This technology has been in continuous commercial operation for nearly 4 years and is currently being deployed at various industrial sites (Steel mills, Petrochem, Gasification sites) around the globe. In May 2018 the first full commercial scale facility was started at a steelmill in China and production results from this plant will be presented. This plant is RSB certified.

In summary, gas fermentation offers an efficient route to add greater value to gas streams than established technologies, while also reducing greenhouse emissions and providing a strategically important alternative to food or farmed resources for domestic production of sustainable fuels and chemicals at an impactful scale.

RSB – Roundtable on Sustainable biomaterials rsb.org

# Roelands | Development of a dissolution process for recovery of polymers with improved quality from waste plastics: status and challenges

Theme **Circularity**
Authors Mark Roelands, Lucie Prins
Affiliation TNO

Dissolution-based recycling technology has the potential to recover purified polymers from waste plastics with improved quality compared to polymers obtained by mechanical recycling only, e.g.

by removal of contaminants and additives that are responsible for odour and colour. At TNO a dissolution process is under development for upcycling of polymers from waste plastics that are hard to recycle, like multilayer packaging films, polymer blends and plastics from waste electronics that contain flame retardants. The dissolution technology aims for the use of a single superheated solvent, to obtain hot polymer solutions with reasonably high concentration for viable process economics and with sufficiently low viscosity to allow for effective use of conventional purification techniques like microfiltration and sorption. Interaction between solvent, polymer and contaminants plays an important role during the development of the technology. Hence process development starts with experimental screening for suitable solvents while subsequently purification methods to remove additives and impurities from polymer solutions are experimentally explored. Next the polymer must be recovered from the solution, either by evaporation of the solvent, by precipitation induced by cooling down or by addition of an anti-solvent. Finally, the polymer must be devolatilized and the solvent recovered for recycling in the process. Currently the process is carried out at a scale suitable to produce approx. 100 grams per day with scale-up started to kg per day. In this lecture the process development methodology will be explained, illustrated with examples from our experience and with references from ongoing development by industry and institutes.

# Schellevis | Direct air capture with a 1 kg/day fixed bed reactor system using solid amines

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| Theme | **Circularity** |
| Authors | H.M. Schellevis and D.W.F. Brilman |
| Affiliation | University of Twente |

Direct Air Capture (DAC) is the extraction of $CO_2$ directly from the atmosphere. This is an important technology in our quest towards carbon neutrality. At the UT, we developed a small scale DAC pilot unit with a productivity of 1-1.5 kg $CO_2$/day. The DAC facility is based on adsorption using supported-amine sorbents in a system with four parallel shallow fixed bed reactors, with a total targeted system productivity of 1 kg $CO_2$/day. A steam-assisted temperature-vacuum swing (TVSA) is used in the regeneration step, where the sorbent remains fixed in the same reactor compartment as during the adsorption. The system is fully automated and uses a time-based process control. The time-based process control implies that each phase has a predefined duration, such that three reactors are in adsorption mode and one is in regeneration mode.

In this study, we present the capture performance of continuous experiments that span multiple days with varying operational parameters (e.g. cycle time and desorption temperature). The system is fed with ‘real’ air that is extracted directly from the laboratory. This means the air feed has small fluctuations in temperature, relative humidity and $CO_2$ concentration. For the base case scenario, the average working capacity is 0.7 mol/kg with leads to a productivity of 0.22 kg $CO_2$/kg sorbent/day and a system productivity of 1.2 kg $CO_2$/day. The energy consumption is approximately 16 MJ/kg $CO_2$ of which 83% is thermal energy and 17% is electrical energy.

# **Veldhuizen** | Tuning $CO_2$ - $H_2O$ Competitive and Cooperative Adsorption through Humidity Control in Covalent Organic Frameworks

Theme **Circularity**
Authors Hugo Veldhuizen, Sybrand van der Zwaag, Monique van der Veen
Affiliation Delft University of Technology

In order to separate and capture $CO_2$ from the air or flue gas streams, the influence of water has to be taken into account, as it hampers the capture process in two main ways: (1) water preferentially binds to $CO_2$ adsorption sites and lowers the overall capacity, and (2) water causes hydrolytic degradation and pore collapse of the porous framework. Here, we have used a water-stable polyimide covalent organic framework (COF) in $N_2$ / $CO_2$ / $H_2O$ breakthrough studies and assessed its performance under varying levels of relative humidity (RH). We discovered that by controlling the RH we were able to steer the competitive binding of $H_2O$ over $CO_2$ in the direction of cooperative adsorption, where RH levels of around 15 % offered additional binding sites. This research offers experimental design rules to optimize $CO_2$ capture performance of nanoporous materials under industrial conditions, while gaining fundamental insights into the driving forces for these adsorbent–adsorbate interactions.

# THEME: Electrifying the Industry

## Bleeker | Pressure swing for gas bubble removal in electrolysis

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| Theme | **Electrifying the industry** |
| Authors | Jorrit Bleeker, David A. Vermaas |
| Affiliation | Delft University of Technology |

Renewable hydrogen production is expected to play a key role in the energy transition. Alkaline electrolysis uses abundant transition metal electrodes to achieve high activity for hydrogen and oxygen evolution, making it a cost-effective water electrolysis technique. The main drawback of alkaline electrolysers is the low energy efficiency at high current densities (&gt;0.2 A/cm2). A large fraction of the energy losses can be attributed to gas bubbles, that partially block the electrode surface and reduce the conductivity of the electrolyte.

To reduce the effects of gas bubbles, electrolysers can operate at elevated pressures (1-50 barg), which significantly reduces the Ohmic resistance. However, over time a larger and larger layer of gas bubbles will block the electrode surface.

In our group we developed the “Pressure swing” as removal method for these surface gas bubbles. By periodically (every 5-600 seconds) reducing the pressure, the surface bubbles will grow in size and are taken of the electrode resulting in a lower average cell voltage, up to 140 mV in current measurements.

## Slotboom | Methane pyrolysis by pulsed compression

Theme **Electrifying the industry**
Authors Yordi Slotboom, Sander Roosjen, Alexander Kronberg, Maxim Glushenkov, Sascha R.A. Kersten
Affiliation University of Twente

The direct coupling of methane to more valuable chemicals like ethylene remains a challenging process. Most processes suffer from low yields and deactivation due to tar and coke formation. If natural gas or renewable biogas could be upgraded to ethylene, the current naphtha feedstock could be replaced. Plastics could be made from cleaner or even renewable sources.

This research uses a novel technology that heats up a gas mixture by means of compression. This is done by the use of a free piston inside a cylinder. Methane feed mixtures can be compressed up to 500 bar and 2000 K. The energy is provided through high pressure nitrogen. It is released underneath the piston, after which it moves up and compresses the feed within 8 milliseconds. These extreme conditions allow for the non-oxidative pyrolysis of methane to mostly ethane, ethylene and acetylene. A benefit of this technology is that the gas mixture is also immediately quenched after the initial compression. This stops the further reaction of the desired products to tar and soot.

Another advantage of this concept is the relatively low reactor and feed temperature of 500 K compared to the gas temperature of 2000 K. This potentially means an energy efficient high temperature process, where the feed can still be heated by electric heaters. Initial experimental results showed a 24% $C_2$ yield at a total of 26% methane conversion without any observable soot [1].

[1] Slotboom, Y., Roosjen, S., Kronberg, A., Glushenkov, M., & Kersten, S. R. A. (2021). Methane to ethylene by pulsed compression. Chemical Engineering Journal, 414, 128821. https://doi.org/10.1016/J.CEJ.2021.128821

# Vos | Towards fossil-free ethylene: ex-ante techno-economic comparison of low TRL technologies

Theme **Electrifying the industry**
Authors Josephine Vos, Paola Ibarra-Gonzalez, Tom Burdyny, Andrea Ramirez
Affiliation Delft University of Technology

Reaching our climate goals requires urgent advancements in fossil-free technologies. Potential solutions for ethylene production could be technologies using alternative raw materials (ARM). This study explored the potential trade-offs of three low technology readiness level (TRL) ethylene production processes from biomass and $CO_2$ via ex-ante techno-economic and environmental analyses. This was done by: (1) comparison of the three processes in terms techno-economic and environmental performance; (2) comparison of these results with the business-as-usual process; and (3) identification of the key bottle-necks to overcome for performance improvement of the three processes.

The results of this study showed that despite significant differences in feedstock and process design between the three routes, no single route significantly outperforms the rest. Also, it was found that the three low TRL routes are not favorable in terms of techno-economic and environmental performance when compared to the business-as-usual scenario under the current modelled assumptions. This study identified all three routes are technologically limited by low conversion of the feedstock into ethylene in the main process sections. Furthermore, it was found the valorization of byproducts is of significant importance. Additionally, as a $CO_2$ mitigation option these three routes are not an effective solution due to low conversion of feedstock into products and large amount of $CO_2$ recycles in the processes.

Key words: ethylene, alternative raw materials, ex-ante techno-economic analysis, process systems engineering, environmental sustainability, low carbon technologies

# THEME: Electrochemical Processing

## Bagemihl | Modelling the Electroreduction of $CO_2$ Under Gas-Liquid Taylor Flow

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| Theme | **Electrochemical processing** |
| Authors | Isabell Bagemihl, Chaitanya Bhatraju, J. Ruud van Ommen and Volkert van Steijn |
| Affiliation | Delft University of Technology |

TU Delft's e-Refinery initiative is aiming to accelerate the shift from fossil-based chemical industry to sustainable electricity-based systems.

Utilising $CO_2$ as a feedstock for electrochemical reduction has the potential to close the carbon cycle while acting as a storage for renewable energy. However, the $CO_2$ electrolysis in aqueous systems is severely limited by mass transfer leading to total current densities insufficient for industrial applications. Current reactor designs overcoming these mass transfer limitations pose challenges for scale-up. Gas liquid segmented flow in micro- and millimetre-scale reactors could overcome these challenges and present a potential design for $CO_2$ electrolysers. However, this reactor concept has only scarcely been studied for electrolysis and the effect of process conditions on the reactor performance are poorly understood. We present a 2D unit cell model to numerically investigate under which conditions this novel reactor concept can be a viable option for the electrochemical reduction of $CO_2$. We show that the total current density in this reactor exceeds > 200 mA/cm$^2$ by reducing the diffusion layer thickness near the cathode by one order of magnitude (Figure 1). High void fractions and low bubble velocity lead to an increase in current density and faradaic efficiency towards CO, which increases with increasing pressure. Further, the CO:$H_2$ ratio is dictated through the superficial velocities at the inlet. The insights of our model will guide practical studies on reactor design and performance.

## Baumgartner | How does the GDE structure affect the resistance against flooding due to hydrostatic pressure differences in $CO_2$ electrolyzers?

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| Theme | **Electrochemical processing** |
| Authors | Lorenz M. Baumgartner, Christel I. Koopman, Antoni Forner-Cuenca, David A. Vermaas |
| Affiliation | Delft University of Technology |

Electrochemical $CO_2$ reduction is a promising process to store intermittent renewable energy in the form of chemical bonds and to meet the demand for hydrocarbon chemicals without relying on fossil fuels.

Researchers in the field have used gas diffusion electrodes (GDE) to supply $CO_2$ to the catalyst layer from the gas phase. This approach allows to bypass mass transfer limitations imposed by the limited solubility and diffusion of $CO_2$ in the liquid phase at a laboratory scale. However, at a larger scale, pressure differences across the porous gas diffusion layer can occur. This can lead to flooding and electrolyte breakthrough, which can decrease the performance. The aim of this study is to understand the effects of GDE structure on flooding behavior and $CO_2$ reduction performance. We approach the problem by preparing GDEs from commercial substrates with a range of structural parameters (carbon fiber structure, thickness, cracks). We then determined the liquid breakthrough pressure and measured the Faradaic efficiency for CO at an industrially relevant current density. We found that there is a trade-off between flooding resistance and mass transfer capabilities that limits the scalability. This trade-off depends strongly on the thickness and the structure of the carbon fiber substrate. We propose a design strategy for a hierarchically structured GDE which might offer a pathway to perform electrochemical $CO_2$ reduction at an industrial scale.

## Ligthart | Suspension electrodes for enhanced mass transfer in electrocatalytic CO2 reduction

Theme **Electrochemical processing**

Authors Nathalie E.G. Ligthart, Johan T. Padding, David A. Vermaas
Affiliation Delft University of Technology

When intensifying electrochemical energy conversion processes that deal with low concentrated reactants (like resource recovery or $CO_2$ conversion),

mass transport limitations occur and cause low Faradaic efficiencies (FE) at high current densities. We investigate whether mass transport can be improved by using flowable suspension electrodes instead of stationary electrodes. In the case of $CO_2$ reduction to CO, $H_2$ evolves as a side product because of slow $CO_2$ transfer, lowering the FE for CO. In this study, we aim to perform $CO_2$ reduction at high current density and FE on a flowable suspension electrode. We use silver nanoparticles as catalyst and suspend them together with electrically conductive and capacitive microparticles in $CO_2$-saturated electrolyte and test the performance of this flowable cathode in a flow cell. Tailoring this system opens up a route to enhanced mass transfer in more electrochemical energy conversion processes.

# THEME: Energy

## **Hadian** | Kinetic study of $CO_2$-free production of carbon nanomaterials and hydrogen from methane in a fluidized bed reactor

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| Theme | **Energy** |
| Authors | M.Hadian, D.P.F.Marrevee, K.A.Buist, B.Reesink, A.N.R.Bos, A.P van Bavel, J.A.M.Kuipers |
| Affiliation | Eindhoven University of Technology |

Global warming obliges us to seek for more sustainable processes without $CO_2$ emissions.

Starting from base chemicals such as methane which can be converted into hydrogen and functional nano carbon materials without emitting greenhouse gases by ThermoCatalytic Decomposition of methane (TCD). The process of growing catalyst particles brings significant complexities. The kinetics of this reaction over a nickel supported catalyst is studied in a fluidized bed reactor. In order to account for these complexities, a special fluidized bed reactor is designed and built. In the experiments a commercial nickel catalyst on a silica support was used and the effect of operating conditions (temperature, concentrations of methane and hydrogen and weight hourly space velocity (WHSV)) was evaluated. Maximum reaction rate, lifetime and carbon yield are used as the performance parameters of the catalyst. Values up to and in excess of 70g of fishbone carbon fibers and 12 h (at 550°C and 70vol.%CH4- 5vol.%H2) have been achieved for carbon yield and lifetime, respectively. Lower temperatures and the presence of a small fraction of hydrogen has a positive effect on the carbon yield and lifetime. While lower concentrations of methane lower the reaction rate, the lifetime and the carbon yield. The dynamic reaction rate over time is modelled by two factors: maximum reaction rate and deactivation factor. The model parameters were estimated for the temperature range of 550 −600°C and it predicts the experimental data with a reasonable accuracy.

## Heijden, van der | Towards bottom-up design of porous electrode microstructures – coupling evolutionary algorithms and pore network modelling

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| Theme | **Energy** |
| Authors | Maxime van der Heijden, Rik van Gorp, Mohammad Amin Sadeghi, Jeffrey Gostick, and Antoni Forner-Cuenca |
| Affiliation | Eindhoven University of Technology |

Porous electrodes are performance- and cost-defining components in electrochemical systems that must facilitate mass transport, provide surfaces for electrochemical reactions, and conduct electrons and heat. Thus, understanding and optimizing the electrode microstructure offers a promising pathway to cost reduction. To accelerate progress, microstructure-informed multiphysics simulations can be leveraged to aid the theoretical understanding and design of advanced electrode architectures. In this work, we explore the following question: Can we deploy three-dimensional simulations combined with evolutionary algorithms to enable bottom-up artificial generation of porous electrodes?

In the first part of this talk, I will discuss the modeling framework and experimental validation. Using a pore network modeling open-access platform (OpenPNM), we built a computationally inexpensive, microstructure-informed, and electrolyte-agnostic simulation framework with the focus on redox flow batteries. The model utilizes a network-in-series approach to account for species depletion over the entire length of the electrode and was validated with symmetric flow cell experiments for two distinct electrolytes (aqueous and non-aqueous) and two types of porous electrodes (carbon paper and cloth). The dry electrode microstructures were obtained with x-ray computed tomography and converted into a network of spherical pores and cylindrical throats. The electrochemical performance of the non-aqueous electrolyte was well captured by the model. For the aqueous electrolyte, we find that incomplete wetting of the electrode results in overprediction of the electrochemical performance, which was accounted for by employing a fitting parameter to account for the near-surface mass transfer coefficient.

In the second part of the talk, I will describe a genetic algorithm that optimizes porous electrode microstructures from the bottom-up by coupling the pore network model with an evolutionary algorithm. The microstructure evolves driven by a fitness function that minimizes pumping power requirements and maximizes electrochemical power output. The analyzed systems show significant improvement of the networks' fitness, which increased by 30%. The presented framework offers great potential for predictive design of electrode microstructures tailored for specific redox chemistries and reactor architectures, which will accelerate and broaden the design and fabrication of advanced electrode structures.

Acknowledgments:
This work is part of the Talent Programme Veni with project number 17324, which is partly financed by the Dutch Research Council (NWO).

# Rahimalimamaghani | The effect of ethylene diamine in ultra selective CMSMs for $CO_2$ separation from natural gas.

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| Theme | **Energy** |
| Authors | A. Rahimalimamaghani, D. A. Pacheco Tanaka, M. A. Llosa Tanco, M. F. Neira D'Angelo, F. Gallucci |
| Affiliation | Eindhoven University of Technology |

Natural gas purification is considered one of the high CAPEX and OPEX processes in the world.

Absorption is used as state-of-the-art technology in separation of $CO_2$ from natural gas to reach the high methane concentration which is a standard for injecting the methane to the natural gas grid due to the damage that $CO_2$ results in terms of corrosion and low heat value per volume unit.

The absorption technology could be substituted with membrane separation which offers scalable, low cost, environmentally friendly and lower energy consumption process. Although polymeric membranes are considered as a potential candidate for the purification of natural gas, the low $CO_2/CH_4$ perm-selectivities and plasticization in high pressures or high concentration of $CO_2$ prevents from further deployment of this technology in industries.

Carbon Molecule Sieve membranes (CMSMs) offering high perm-selectivity properties and stable performance at high operational pressures, in presence of $H_2S$ and high concentrations of $CO_2$. CMSMs outperform polymeric membranes according to the Robeson's upper bound limit according to literature data. In this work the supported CMSMs are synthesized from resorcinol- formaldehyde resin and the $CO_2/CH_4$ perm-selectivity is enhanced by introduction of amine functional groups in the carbon matrix. Ultra $CO_2$ selective membranes are fabricated and tested for their performance in terms of permselectivity and stability at high pressures up to 55 Bar.

# Saedy | Correlating the co-catalyst loading and the activity of $TiO_2$ photocatalyst

Theme **Energy**
Authors Saeed Saedy, Nico Hiemstra, Dominik Benz, Hao Van Bui, J. Ruud van Ommen
Affiliation Delft University of Technology

Harvesting solar energy is a promising solution for the mitigation of $CO_2$ emission and the energy transition from fossil fuels to renewable energy.

Photocatalysts can harvest solar energy directly and store it in chemical bonds via processes such as solar hydrogen production. Well-engineered photocatalysts are crucial for these processes, and the large-scale production of an efficient and inexpensive catalyst can pave the way for industrial solar hydrogen production. $TiO_2$ shows an excellent potential for large-scale application as photocatalyst; however, it suffers from its limited activity to UV-light. The doping and decoration of $TiO_2$ with small band-gap semiconductors can boost its activity. However, obtaining the optimum amount/size of co-catalyst is a challenge for maximizing the photo-activity of $TiO_2$ in a cost-effective way. We deposited $CuO_x$ nanoparticles on AEROXIDE® P25 $TiO_2$ using atomic layer deposition. The $CuO_x/TiO_2$ samples were obtained with Cu loading of 0.7-4.8 wt.%, which the average $CuO_x$ size of samples with Cu content up to 3.8 wt% was about 1.7 nm. These samples showed significant $H_2$ productivity improvement compared to pure P25. The results allowed us to correlate the loading of CuxO clusters to the photoactivity of $CuxO/TiO_2$ and develop a model to describe the $CuO_x/TiO_2$ photo-activity as a function of $CuO_x$ loading. This model enables us to predict the optimum $CuO_x$ loading of the $CuO_x/TiO_2$ system for different particle sizes, and can be employed for optimizing the co-catalyst loading for photocatalytic processes, facilitating the photocatalyst design/production process.

## THEME: Materials Processing & 3D Printing

### Botto | Flow processing of graphite and carbon materials: how to make valuable products from waste carbon

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| Theme | **Materials processing & 3D printing** |
| Authors | Lorenzo Botto, Catherine Kamal, Adyant Agrawal, Hugo Perrin, Simon Gravelle |
| Affiliation | Delft University of Technology |

Carbon can be an extremely useful material and its rational processing a key enabler for the energy transition. While the harmful effects of gaseous carbon on the atmosphere has given “carbon” a bad publicity, one should not forget that carbon is a key element of the batteries that will power our future.

In this talk, I will overview our experiences with understand the fluid dynamics of carbon, which we achieve through a combination of theory and experiments. Particularly, I will highlight our recent research aimed at understanding fundamentals the liquid-phase exfoliation process to produce high-value graphene from commonly available graphite or waste graphitic carbon. From a fluid dynamics standpoint, the phenomenon of exfoliation is fascinating and involves an interplay of flow phenomena, adhesion and fracture mechanics, which we unveil with high-resolution simulations. With fine control, liquid-phase exfoliation could be used to produce sheet like nanoparticles from all layered crystal materials, offering the possibility of revolutionising the production of high-performance fibers, nanocomposites and lubricants.

The final goal of our research efforts developing the next generation models to predict the implementation of large-scale exfoliation for the production of graphene and other 2D materials on the ton scale required by market applications.

Finally, I will also share our recent first experiences in designing the rheology of carbon inks made of biochar particles. The key design challenge is to optimise the compromise between yield stress and flowability, to obtain an ink that can be used in 3D printers and molding processes to make completely degradable biochar-based products.

## Mularczyk | Synthesis of electrode materials for electrochemical devices using dynamic hydrogen bubble template deposition

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| Theme | **Materials processing & 3D printing** |
| Authors | Adrian Mularczyk, Antoni Forner-Cuenca |
| Affiliation | Eindhoven University of Technology |

Distributing liquid or gaseous chemicals from flow channels to a catalyst layer is common in many chemical and electrochemical applications where, especially in the latter, the use of porous, carbon fiber based structures has become prevalent. Over the years, many shortcomings of plain fiber based structures have come to light. For example, in fuel cell and electrolysis applications, the incorporation of a reduced pore size on the side facing the catalyst layer resulted in significant improvements to performance1,2. Furthermore, the counterflow of multiple phases (gas and liquid) in the form of reactants and products results in highly complex and suboptimal transport situations inside the electrodes. This motivated the development of materials with dedicated pathways for both phases and which have been investigated in the form of chemical3 and geometrical4,5 alterations of the carbon fiber material. While these adaptations succeed at improving the performance of the base material, it would be desirable to directly synthesize a material that features a pore size gradient as well as dedicated pathways for different phases.

To address this issue we propose the use of metal foams generated with dynamic hydrogen bubble templating6,7. Their bimodal pore size distribution and intrinsic pore size gradient combined with a simple formation procedure make them an interesting candidate for the application in electrochemical devices. Obtaining a self-standing version of this material is however non trivial as it is attached to the base substrate used to generate it. Leveraging a novel method to overcome this limitation we are able to generate this structure in a self- standing form, suitable for the use in electrochemical devices. In my lecture I will give a general overview of the formation process and discuss the relationship between the deposition parameters and the resulting micro structure of the material in terms of porosity, thickness and pore size.

# Perrin | Buckling of sheets in liquids to understand liquid-phase processing of two-dimensional materials

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| Theme | **Materials processing & 3D printing** |
| Authors | Hugo Perrin, Heng Li, Lorenzo Botto |
| Affiliation | Delft University of Technology |

2D nanomaterials such as graphene and 2D polymers have attracted much attention as key enablers in applications ranging from nanocomposites, energy generation devices to biomedicine. Applications such as printing of conductive inks, production of foams to make porous materials, and film coating techniques require processing 2D nanomaterials in liquids, where the presence of a flow can cause 2D nanomaterial particles to buckle, changing particle morphology and therefore material properties. To analyze the effect of particle interactions on the buckling process, we performed an experimental study on a model system composed of thin Mylar sheets suspended in simple shear flow. This system is designed to replicate on macroscopic scales the mechanics of real graphene. We can vary systematically the distance between sheet pairs, the bending rigidity and the shear rate. We could measure the critical non-dimensional shear rate for which a graphene sheet buckles. Surprisingly, we found that the critical shear rate to bend a pair of close sheets is lower by up to a factor of 10 compared to an isolated sheet. A fluid mechanical analysis reveals that this effect is due to the dipolar flow caused by the neighboring particle, which produces a lateral load on the first particle. For smaller separations, lubrication forces start to prevail, and the relation between distance and critical shear rate for buckling becomes non-monotonic. These results suggest that the buckling threshold in a sheared suspension of sheet-like particles is not purely a material property, but depends sensitively on the particle concentration. (ERC grant. N.715475 acknowledged).

# Rosseau | Enhanced heat transfer by cross flow-inducing catalyst structures: additive manufacturing leads to process intensification

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| Theme | **Materials processing & 3D printing** |
| Authors | Leon R.S. Rosseau, Jord T.A. Jansen, Ivo Roghair and Martin van Sint Annaland |
| Affiliation | Eindhoven University of Technology |

The additive manufacturing, or 3D-printing, of catalyst materials allows for the structuring of catalytic packed bed internals with a degree of design freedom that cannot be achieved through conventional methods. Many of the present literature in this field considers so-called ‘logpile structures’ which consist of stacked cylindrical features. These structures are mostly isotropic and resemble honeycomb monoliths. Due to this similarity, it is to be questioned whether such structures exploit the opportunities of additive manufacturing to the fullest degree, and whether this enables reactor engineering benefits over conventional packed bed reactors. The latter is a requirement for application of this novel catalyst structuring technology, since in its current state, it is more expensive than conventional methods and the catalyst dilution due to significant quantities of binder need to be compensated for.

Hence, novel 3D-printed structures need to realize process intensification to provide quantitative benefits that demonstrate their viability. One process intensification strategy that is envisioned is to increase the wall-to-bed heat transfer rate. This can be done by either of two options: the use of a conductive structure or anisotropic structuring to enable a higher degree of transverse dispersion. The second option is deemed promising since the entire structure can be catalytically active, and this benefits kinetically-limited reactions.

The concept of anisotropic structuring can be envisioned as macroporous baffles within the structure which steer the fluid flow towards the wall in a cross flow-like regime. The intense contact with the wall should benefit wall-to-bed heat transfer rates. The penalty for this enhanced heat transfer is a higher pressure drop. By changing the properties of the structure, these phenomena can be balanced and flexible operating windows for chemical reactors can be obtained.

In this oral presentation, we discuss our experimental efforts which demonstrate the tunability of transport properties in isotropic logpile structures. These results show that by changing the geometry of the structure, the degree of transverse dispersion can be varied within a relatively limited range of values. To expand this range, several designs of anistropic logpile structures are proposed. The potential for intensified heating thanks to cross flow operation in these novel structures is evaluated using modelling in OpenFOAM. The effect of the design parameters of the structure on the thermal management and residence time distribution will be discussed, including considerations on the viability of implementation of these structures in reactive applications.

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# THEME: Process Systems Engineering

## **Huynh** | Superstructure optimization for biodiesel production: from feed to fuel

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| Theme | **Process Systems Engineering** |
| Authors | Thien An Huynh, Mattia Rossi, Maryam Raeisi, Meik B. Franke, Flavio Manenti, Edwin Zondervan |
| Affiliation | University of Twente |

Biodiesel, derived from renewable biobased feedstock, is considered a cornerstone in the EU strategy to reduce the use of fossil fuels in transportation. It had a share of 74% the total renewable energy used in the EU transport sector in 2020. However, the public perception of bioeconomy is changing, i.e., the growth of biofuel has been slowing down recently with an increase of only 6.8% from 2018 to 2019 because of its high production cost and the change for non-food feedstocks.

While there are many studies which focus individual challenges, between finding inexpensive feedstocks and developing optimal processes for biodiesel production, a combined strategy has not received enough attention. Therefore, this work fills the gap of knowledge by systematically combining the selection of appropriate feedstocks and innovative technologies into a superstructure model for biodiesel production optimization.

A superstructure model for maximizing the profit of biodiesel production is presented in this work. The superstructure encompasses a wide range of feedstocks (e.g., waste cooking oil, tallow, rapeseed oil and algae), conventional reaction and separation equipment (e.g., continuous stirred tank reactor, decanter and vacuum distillation) and intensified operation units such as membrane reactor and reactive distillation column. The superstructure model is implemented in Advanced Interactive Multidimensional Modeling (AIMMS). The results present an optimal design of a biodiesel production process from waste cooking oil and tallow with a heterogeneous acid catalyst, a reactive distillation column and additional purification steps for producing pure glycerol which is 40% higher in price than technical glycerol. The total annual profit of the biodiesel production from waste cooking oil is 828,697 USD and from tallow is 976,450 USD. The results show that the combination of feedstock selection and implementation of advanced processing technologies to improve biodiesel production can be achieved with the superstructure optimization method.

# Noll | Economic comparison of reactive distillation (RD) to a benchmark conventional flowsheet: regions of RD applicability and trends in column design.

Theme **Process Systems Engineering**
Authors Lionel Noll
Affiliation University of Twente

Reactive Distillation (RD) is one of the most prominent examples of Process Intensification. Nonetheless, a distillation column is an inefficient vessel for holding large liquid holdups, such that applications requiring significantly large residence times could prefer a dedicated reactor and separation train. Knowledge of the limits of RD applicability is an important step towards structurally incorporating RD within process synthesis.

We present a methodology that benchmarks RD against a conventional reactor + distillation train flowsheet based on their cost-optimized designs. The developed optimization framework includes established correlations for tray hydraulics, enabling the design of cost-optimized reactive internals.

This methodology is applied to an ideal liquid phase reaction A+B↔C+D with boiling point order T_C^Boil<T_A^Boil<T_B^Boil<T_D^Boil, for all relevant combinations of reaction rate, chemical equilibrium and VLE. The resulting flowsheet regime map for this general class of chemical systems indicates that a very large economic potential for RD exists if a reactant/product separation is difficult to achieve with conventional distillation (αreactant-product approaches 1.2) and reaction rates are moderately limiting at most.

Key design strategies to allow for sufficient reactive liquid holdup that were identified are the choice of using bubble-cap trays, higher than conventional weir heights and most strikingly the deliberate overdesign of column diameter, operating at 40% of flooding gas velocity, to create physical space on the tray for the liquid froth and maximizing the effective froth density.

The established regime maps and RD column designs can serve as tools to aid flowsheet synthesis and provide a tangible starting point for RD column and tray design.

# Raeisi | Sustainable design of microalgae biorefinery to produce added-value products

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| Theme | **Process systems engineering** |
| Authors | Maryam Raeisi, Meik B Franke, Edwin Zondervan |
| Affiliation | University of Twente |

Microalgae are a promising feedstock not only for biofuels production but also for various added-value products. However, extraction and purification bioproducts from microalgae is a cumbersome task and very expensive. Thus, this is a big challenge for several industries in the Netherlands and others around the world.

Although there have been various studies regarding the production of biodiesel from algae, the identification of cost-effective pathways for producing these bioproducts is structurally lacking. Developing and optimizing superstructure is one way to develop this sustainable feedstock for many applications. In this work, a superstructure of microalgae biorefinery is developed to produce pigment, omega-3, glycerol, biodiesel, biofuel, and fertilizers from Chlorella Vulgaris, Haematococcus Pluvialis, or Nannochloropsis spp. Two types of wastewaters (influent and wheat straw biorefinery) have been chosen to consider the role of water and nutrients on optimizing pathways and annual profits of microalgae biorefinery.

The superstructure is converted to mixed non-linear programming (MINLP) models to find a cost-effective pathway. Among more than 1100 pathways, the optimized superstructure chose open pond, sedimentation, flotation, flocculation/ centrifugation, sonication, organic solvent-based pigment extraction, n-butanol based lipid extraction, anaerobic digestion. The type of microalgae does not have any role in the chosen pathway. In contrast, the type of wastewater defines the technologies of the dewatering step (flocculation/ centrifugation). Haematococcus Pluvialis biorefinery when using influent wastewater has the most profits. This microalgae biorefinery can have 107 million Euros income annually using 0.2 million tons wastewater.

# Rizki | Model-based optimization of protein purification in multistage ultrafiltration

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| Theme | **Process Systems Engineering** |
| Authors | Zulhaj Rizki, Ruud van Beckhoven, Richard Ravesloot and Marcel Ottens |
| Affiliation | Delft University of Technology |

Ultrafiltration has become a common technique to purify protein from its native mixture. Here, the protein is collected at the retentate stream where the impurities are washed and collected in the permeate stream. Having this condition, the protein purification is hardly satisfactory with a single pass ultrafiltration. Repeated diafiltration processes are commonly coupled with the ultrafiltration making it a multistage ultrafiltration/diafiltration (UF/DF) system. While allowing us to have a higher purity protein, a standard UF/DF set up has a major disadvantage related to a large amount of water requirement. Another attempt to improve the standard UF/DF design is to recycle the permeate streams giving similar dilution effect from diafiltration. This creates a counter-current cascaded ultrafiltration system. While this design may greatly reduce the water consumption, the treatment may affect the product outcomes. To solve that dilemma, a sufficient optimization tool is needed to be able to select the optimum configuration and operating conditions.

Optimization of such protein purification system can be formulated as a non-linear programming (NLP) problem with a superstructure. The superstructure represents all alternative configurations, including the standard UF/DF, the complete recycled cascade and the hybrid one. The optimum combination of operating conditions will also be solved simultaneously in this optimization.

This presentation will show the development, nature and performance of the optimization model. The optimization model is developed sequentially starting with modelling a single ultrafiltration process, growing to a multistage system then formulating them into an optimization problem. The protein ultrafiltration is a dynamic process, thus a dynamic model is developed to capture the time dependency. The membrane flux over time is modelled using the cake formation approach. The model also considers the concentration polarization and other mass transfer phenomena. The cake properties are fitted from experimental data. Using such parameters, the model is able to simulate the performance of both single stage and multistage ultrafiltration system. This model is later suitable to be used in the optimization model. Finally, the optimization model is solved using a global optimizer (e.g. genetic algorithm).

# THEME: Transport Phenomena/Reactor Engineering

## Boz | Conformal PEDOT/PSS coatings on porous electrodes for flow through deionization batteries

Theme **Transport phenomena/Reactor engineering**
Authors Emre Burak Boz, Marcell Fritz, Marjolein Boom, Kitty Nijmeijer and Antoni Forner-Cuenca
Affiliation Eindhoven University of Technology

Heavy metal pollution is a developing environmental problem[1] and decarbonization technologies contribute to this problem by driving the demand for rare and heavy metals[2].

Toxic heavy metals are found in their ionized form in wastewaters and are usually in low concentrations. These properties make electrochemically-assisted ion-immobilization technologies attractive platforms for their separation. The immobilization of ions in these technologies occur by balancing the surface charge of the electrode material. Existing flow electrochemical platforms such as fuel cells and electrolyzers benefit from macroporous electrodes that supply the surface area for reactions and boost convective transport for fluids. However, ion-immobilizing electroactive layers are difficult to deposit on such 3D electrode structures as these materials are often non-conductive and require a conductive carrier matrix. Conductive polymers offer an inherent advantage as they can be electropolymerized on complex architectures and can provide a conductive matrix for ion-exchange materials. We hypothesize that, by coupling convection enhanced flow cell designs[3] and porous electrodes with ion-selective coatings[4], we can realize continuous ion separation with improved energy efficiency and short cycle times.

In this work we investigate the applicability of poly(3,4-ethylenedioxythiophene)/ poly(sodium-4-styrene sulfonate) (PEDOT/PSS) on commercial carbon fiber-based paper electrodes through electropolymerization. PEDOT acts as the redox-active component that allows switching of the surface charge with a potential control while PSS acts as the cation-exchange component. In this way we fabricated a 3D-structured, macroporous and electrochemically switchable ion-exchange electrode. We explored the morphology of several PEDOT coatings and show that the PEDOT/PSS system has affinity towards cations due to the PSS in the structure. We revealed transport limitations within the polymer layer where thinner coatings have highest $Ni^{2+}$ adsorption capacity, but thicker coatings are more selective towards $Ni^{2+}$ than $Na^{+}$. Separation cells with flow-through flow design have been constructed with symmetric PEDOT/PSS coated porous electrodes and an anion exchange membrane. This mechanism, also known as rocking chair[5], allow continuous diluate and concentrate generation, eliminating the need of regeneration cycles. Initial tests show that separation of cations is possible under low applied voltages (≤1 V) and energy recovery is possible owing to the charge/discharge of PEDOT.

# Garcia Llamas | Collision of dense and viscous droplets using the Local Front Reconstruction Method (LFRM).

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| Theme | **Transport phenomena/Reactor engineering** |
| Authors | C. (Cristina) García Llamas, B.A.G. (Bart) Timmermans, M.W. (Maike) Baltussen, K.A. (Kay) Buist, J.A.M. (Hans) Kuipers |
| Affiliation | Eindhoven University of Technology |

Droplet-droplet interactions of liquids with a high solid content or viscosity are critical in a broad range of industrial applications, such as spray drying, fuel combustion or spray coating. The efficiency of these processes depends heavily on the surface area and volume of the droplets after they collide. Thus, it is of foremost importance to accurately describe the physical mechanisms leading to the merge and break-up of droplets. Nonetheless, profound knowledge on the forces dominating the collision is limited, particularly when the liquids have a high solid content or viscosity. In this research, we investigate the capabilities of the Local Front Reconstruction Method (LFRM) in combination with a Direct Numerical Simulation (DNS) to reproduce the collision of two droplets. Four collision regimes are studied (i.e., coalescence, bouncing, reflexive and stretching separation) using three different glycerol solutions. We assess the capabilities of the LFRM by qualitatively comparing the positions of the colliding droplets before and after they touch with the experimentally obtained results at the same conditions.

## Kamphorst | Stirrer design for improved fluidization of cohesive microsilica

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| Theme | **Transport phenomena/Reactor engineering** |
| Authors | Rens Kamphorst, Kaiqiao Wu, Jasper Ford, Gabrie M.H. Meesters and J. Ruud van Ommen |
| Affiliation | Delft University of Technology |

Fluidization can be used for the processing of powders or as a reactor type for chemical reactions.

When it comes to powders with a small particles size, fluidization becomes hard due to strong attractive inter-particle forces. This results in channel formation and agglomeration, both of which undermine fluidization. Throughout the years, several techniques have been developed, often referred to as assistance methods, which allow for improved fluidization of cohesive powders. Mechanical vibration, electric fields, pulsed flow and acoustic vibration have all been shown to improve the quality of fluidization. When it comes to scaling up the reactors, utilizing these techniques, with exception of pulsed flow, becomes increasingly hard. In literature, only a couple of studies were found on the effect of stirring, or mechanical agitation, on the fluidization quality of cohesive powders. And no literature on stirrer design was found at all.

In our study, we look at the effect on fluidization quality of several stirrer parameters. Blade diameter, blade thickness, blade angle, blade orientation and the use of a helix design were all studied. The stirrers were 3D printed and tested in a 5cm column where bed height and pressure drop were measured. As cohesive powder, we used 10µm silica particles.

Results have shown a significant improvement of fluidization quality when stirrers are used. When no assistance is utilized at all, channels are formed and no fluidization takes place. Using a stirrer at a low height disrupts the channel formation and allows the powder to fluidize with a normalized pressure drop of up to 0.9 and bed height expansion ratios of around 1.5, which is comparable to our earlier study on the effect of vibration.

## Kordnejad | Hydrodynamics of a gas-solid fluidized bed with charged particles

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| Theme | **Transport phenomena/Reactor engineering** |
| Authors | Marzieh Kordnejad, Ivo Roghair, Martin van Sint Annaland |
| Affiliation | Eindhoven University of Technology |

The hydrodynamics of a gas-solid fluidized bed with electrostatically charged particles has been investigated in detail by experiments and modeling.

Modeling was done using the Discrete Particle Method in combination with Coulomb's law to determine the electrostatic forces between particles. The model can in principle account for all the electrostatic interactions between all the particles throughout the entire domain and accurately , but this is computationally prohibitively expensive. Conventionally, a cut-off distance is defined and interactions beyond this cut-off distance are neglected, but it was found that this approach results in large inaccuracies in the computation of the electrostatic forces. To tackle this challenge, a hybrid technique was developed that includes both short and long range electrostatic interactions. The short-range interactions are evaluated with Coulomb’s law. On the other hand, for the long-range interactions, the hybrid method regards multiple particles as a single point for the computation of the electrostatic force, basically regarding an equivalent particle that represents a collection of particles located in a cell. The hybrid model affectly achieves an optimum in the trade-off between accuracy and computational efficiency. Using this model, the effect of electrostatic charges on the minimum fluidization velocity, particle motion and bubble size in a small gas-solid fluidized bed were studied.

In addition, experiments were performed using glass particles in a pseudo 2D fluidized bed for both charged and uncharged particles. Comparison between the fluidization onset in an uncharged and charged bed revealed an increase in the minimum fluidization velocity in case of a charged bed. This increase is caused by the repulsive force between the particles, which increases the bed voidage. Therefore, it allowed the system to operate as a fixed-bed at higher gas velocities. Single bubble injection experiments were performed in combination with high-speed imaging, and these image recordings have been analyzed using digital image analysis.

# Liu | Mass transfer in Pickering emulsions for biphasic catalysis

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| Theme | **Transport phenomena/Reactor engineering** |
| Authors | Yanyan Liu, Mingjun Xu, Aza Alawi, Luis Portela, Ruud van Ommen, Valeria Garbin |
| Affiliation | Delft University of Technology |

Pickering emulsions (stabilized by nanoparticles instead of molecular surfactants) are increasingly finding applications in biphasic catalysis.

The catalyst can be on the nanoparticles, or within the emulsion droplets; reaction products are immediately removed from the reaction site at the liquid-liquid interface, giving high conversion and selectivity. The overall performance relies on the efficient mass transfer of reactants/products across the liquid-liquid interface and the interfacial layer of particles. While the nanoparticles help in stabilizing the emulsion, they can also limit the transfer of solutes. The bottleneck in predicting the optimal conditions is our limited understanding of diffusion in Pickering emulsions. To fill this gap, we quantify the diffusive transport of a fluorescent solute and the acid-base neutralization across the interface of a Pickering droplet, together with computational simulations, we established the effects of liquid properties, sizes and surface coverages of the nanoparticles, on mass transfer at a liquid-liquid interface. By comparing with bare droplets, we link the microscopic properties of the particles/droplets and their dynamics, to the mass transfer performance. Such insights will ultimately contribute to control the performance of Pickering-emulsion catalysis, paving the way towards optimized handling of complex, multiphase systems in continuous-flow Pickering emulsion.

# Zong | Effect of nanoparticle addition on the mass transfer of gas-liquid slug flow in microreactors

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| Theme | **Transport phenomena/Reactor engineering** |
| Authors | Jie Zong and Jun Yue |
| Affiliation | University of Groningen |

Microreactor technology has shown promising applications in a variety of multiphase operations, as it can provide much faster heat and mass transfer rates than conventional reactors. Nanofluid (which can be treated as a pseudo single phase) is a new class of fluid that contains the stably dispersed nanoparticles (e.g., $TiO_2$, $Al_2O_3$ and $SiO_2$; particle size on the order of ca. 1-100 nm) with a higher thermal conductivity than the base fluid. Therefore, nanofluid emerges as a potential alternative working fluid in microreactors regarding heat transfer and catalytic reactions (i.e., when nanoarticles function as highly efficient catalysts). In this work, experimental investigations have been performed on the flow and mass transfer during $CO_2$ absorption by nanofluids (e.g., $Al_2O_3$-$H_2O$) through capillary microreactors. Especially the effect of nanofluid concentration, nanoparticle size and gas-nanofluid two phase flow ratio on the overall liquid side volumetric mass transfer coefficient (kLa) and pressure drop were studied systematically. The obtained results will be explained based on the changes in the local flow pattern details in slug flow (e.g., slug/bubble length), fluid properties and capacity of gas absorption enhanced by the local mass transfer mechanisms (e.g., the shuttle effect) due to the addition of nanoparticles.

# THEME: Water Processing

## Lompe | Smaller faster better? Grain size dependent performance of granular activated carbon for organic micropollutant removal

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| Theme | **Water processing** |
| Authors | Nan Jiang, Bas Heijman, Luuk Rietveld, Kim Maren Lompe |
| Affiliation | Delft University of Technology |

Granular activated carbon (GAC) contactors operated with 12 to 20 min empty bed contact time are commonly used for trace organic pollutant removal from drinking water. However, the typically large GAC contactors are costly and not flexible with respect to variable influent concentrations. Reducing the grain size of GAC accelerates adsorption kinetics and could thus allow for shorter EBCT and smaller, more flexible GAC contactors.

Grain size dependent adsorption performance was tested for 10 organic micropollutants spiked in groundwater with low clogging potential. Adsorption isotherms and kinetics were obtained from batch experiments and breakthrough curves were recorded in small-scale laboratory GAC columns over a period of 2 months. A solute transport model was parametrized based on batch adsorption tests to predict breakthrough at full scale. The results from the column studies show that reducing the grain size of GAC from 1,0 – 1.4 mm to 0,5 - 0,8 mm delayed breakthrough by 25 – 30 % depending on the pollutant and without significant pressure build up. The modelling study suggests that a contactor could be operated at a higher flow rate or shorter bed depth (EBCT 5 min) with smaller grains and obtain similar breakthrough performance as a traditional contactor (20 min EBCT).

# Shang | Artificial neural network and genetic algorithm as a hybrid method for optimization of reaction performance and estimation of wastewater component synergistic effect: photocatalytic degradation of ofloxacin antibiotic wastewater using TS-1/$C_3N_4$ composite photocatalyst as a case study

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| Theme | **Water processing** |
| Authors | Qiaoyan Shang, Xiaojuan Liu, Mingfei Zhang , Wenge Liu, Xifeng Shi, Bo Tang, Jun Yue |
| Affiliation | Groningen University |

The preparation of catalysts and the screening of reaction conditions are crucial technologies in the catalysis process. Synthesis conditions of catalyst and optimization of reaction parameters consumes manpower and material resources. In order to solve this problem, with the development of artificial intelligence, researchers began to try to use artificial intelligence methods to simulate the catalytic process. In this work, artificial neural network (ANN) and genetic algorithm (GA) are used as tools for optimization of reaction performance and estimation of wastewater component synergistic effect, taking photocatalytic degradation of ofloxacin (OFX) as a case study. Initially, TS-1/$C_3N_4$ composite was synthesised and used for the photocatalytic degradation of OFX under various experimental parameters. Then, the responding artificial neural network (ANN) models were proposed based on the experimental data. Genetic algorithm (GA) method was used to optimize experimental parameters. Moreover, the influence of wastewater constituents on the RE was investigated by experiment and model. The model can be applied for optimizing reaction processes, analysing the relative importance of parameters and predicting the collaborative influence of wastewater impurities. The good estimation ability of the proposed ANN model has been verified by confirmatory experiments in the presence of cations, metal ions and anions. The responding absolute relative deviation (ARD %) was 6.88 %, 1.04 % and 1.77 %, respectively. It is promising that this research strategy will be extended to the optimization of reaction conditions in photocatalytic microreactors.

# Poster Presentations

## Baumgartner | How does the GDE structure affect the resistance against flooding due to hydrostatic pressure differences in CO2 electrolyzers?

Authors Lorenz M. Baumgartner, Christel I. Koopman, Antoni Forner-Cuenca, David A. Vermaas
Affiliation Delft University of Technology

Electrochemical $CO_2$ reduction is a promising process to store intermittent renewable energy in the form of chemical bonds and to meet the demand for hydrocarbon chemicals without relying on fossil fuels. Researchers in the field have used gas diffusion electrodes (GDE) to supply $CO_2$ to the catalyst layer from the gas phase. This approach allows to bypass mass transfer limitations imposed by the limited solubility and diffusion of $CO_2$ in the liquid phase at a laboratory scale. However, at a larger scale, pressure differences across the porous gas diffusion layer can occur. This can lead to flooding and electrolyte breakthrough, which can decrease the performance. The aim of this study is to understand the effects of GDE structure on flooding behavior and $CO_2$ reduction performance. We approach the problem by preparing GDEs from commercial substrates with a range of structural parameters (carbon fiber structure, thickness, cracks). We then determined the liquid breakthrough pressure and measured the Faradaic efficiency for CO at an industrially relevant current density. We found that there is a trade-off between flooding resistance and mass transfer capabilities that limits the maximum GDE height of a flow-by electrolyzer. This trade-off depends strongly on the thickness and the structure of the carbon fiber substrate. We propose a design strategy for a hierarchically structured GDE, which might offer a pathway to an industrial scale by avoiding the trade-off between flooding resistance and $CO_2$ reduction performance.

# Boulif | Clay composite membranes for salinity gradient batteries

Authors Nadia Boulif, Zandrie Borneman, Kitty Nijmeijer
Affiliation Eindhoven University of Technology

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, the 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 which combine a cheaper hydrocarbon matrix than the state-of-the-art perfluorosulfonated polymers with the attractive properties of inorganic fillers. In this work, composite membranes made of sulfonated poly(ether ether ketone) (SPEEK) and 1 to 20 wt.% aluminum pillared MMT (Al-pil MMT) are considered.

The ion exchange capacity (IEC) of the membranes decreases with an increasing clay loading fraction due to the clays IEC being 10 times lower than that of the SPEEK matrix. Despite the IEC trend, the water uptake of the composite was not influenced by the clay loading owing to the hydrophilicity of the clays. The resulting lower charge density of the composite membranes makes their permselectivity less than 3% lower than that of the SPEEK membrane. Notwithstanding their lower IEC, the conductivity of the membranes increases with an increasing clay loading fraction, reaching up to 1.5 times that of SPEEK for the 20 wt.% Al-pil MMT composite. This is attributed to the creation of percolating sodium diffusion pathways along the flat 2D surfaces of the clays throughout the membrane starting from 5 wt.% clay.

# Chaudhuri | Intensification of the Transesterification Reaction: Scale-Up and Solids Handling

Authors Arnab Chaudhuri, Erdem B. Temelli, Christianus J.W.Hop, Vishnu P. Sureshkumar, John van der Schaaf
Affiliation Eindhoven University of Technology

Fatty acid methyl esters are extensively used compounds in the industry, but perhaps, they are most widely known for their application as biodiesel. In this study we propose the rotor-stator spinning disc reactor (RS-SDR) as an intensified reactor for the production of fatty acid methyl esters. The RS-SDR relies on the generation of high shear forces in the small gap of a disc rotating at high speeds and a stationary wall to improve upon mass and heat transfer rates. Here, we have illustrated the benefits of mass transfer intensification for this reaction by performing the homogeneous base catalyzed reaction in both a single stage and a scaled up multistage RS-SDR. A high level of productivity could be obtained in the multistage reactor ( 7.78 x 103 molmR¬−1 min−1), illustrating the ease of scale up in the RS-SDR and potential for future industrial implementation. Furthermore, we also performed a heterogeneous transesterification reaction with sodium silicate as a slurry catalyst and were able to obtain 72 % conversion in the RS-SDR with a residence time of 8 minutes (productivity of 185 mol mR−1 min−1). In comparison, the batch heterogeneous system had 47 % conversion during the same period of operation time. Despite using high slurry concentrations (up to 20 wt.%), we did not observe any clogging/fouling issues in the reactor. The results here demonstrate the potential of the RS-SDR for not only the transesterification reaction, but also similar reactions which are multiphase in nature.

# Daatselaar, van | Chemical recycling of plastic waste: from polyolefins to short alkanes via hydrogenolysis

Authors Ir. E. van Daatselaar, dr. M.P. Ruiz Ramiro, dr.ir. A.G.J. van der Ham, prof.dr. S.R.A. Kersten
Affiliation University of Twente

Every year, enormous amounts of plastic are produced and used. A significant amount consists of polyethylene (PE) and polypropylene (PP) since feedstock is cheap and applications are versatile. These polyolefins are mainly used for single-use plastics, and the resulting plastic waste is only partly collected and reused as landfill, burned for energy recovery, or recycled.

In this work, it is researched if hydrogenolysis can be implemented to convert polyolefins into valuable products or a feed to the existing steam crackers. In literature, it is shown that converting polyolefins over a ruthenium/carbon catalyst in a hydrogen atmosphere into liquid products is possible. From this previous work, it is found that the batch reaction requires 16 hours for converting a maximum of 1.4 grams of clean, pure polyethylene completely into gas and liquid alkanes at relatively mild reaction conditions. These timeframes, however, are not (economically) feasible for larger-scale processes.

This research elaborates on the first steps into upscaling and implementing the hydrogenolysis reaction. The current experimental results show full conversion of paraffin wax (Mw ≈ 560 Da) and LDPE (Mw ≈ 4000 Da) into gas and short alkanes ($<C25H52$) within 6 hours at 250°C and 40 bar $H_2$ in the presence of Ru/C (1:28 w/w catalyst to polymer). Significant yields of gas and liquid alkanes are reached at shorter reaction times, showing that implementing smart reactor and process design could increase the feasibility of this process.

# Fan | Coupling mesoscale transport to catalytic surface reactions in a hybrid model

Authors Rong Fan, Parsa Habibi, Johan T. Padding, and Remco Hartkamp
Affiliation Delft University of Technology

In heterogeneous catalysis, reactivity and selectivity are not only influenced by chemical processes occurring on catalytic surfaces but also by physical transport phenomena in the bulk fluid and fluid near the reactive surfaces. Because these processes take place at a large range of time and length scales, it is a challenge to model catalytic reactors, especially when dealing with complex surface reactions that cannot be reduced to simple mean-field boundary conditions. As a particle-based mesoscale method, Stochastic Rotation Dynamics (SRD) is well suited for studying problems that include both microscale effects on surfaces and transport phenomena in fluids. In this work, we demonstrate how to simulate heterogeneous catalytic reactors by coupling an SRD fluid with a catalytic surface on which complex surface reactions are explicitly modeled. We provide a theoretical background for modeling different stages of heterogeneous surface reactions. After validating the simulation method for surface reactions with mean-field assumptions, we apply the method to non-mean-field reactions in which surface species interact with each other through a Monte Carlo scheme, leading to island formation on the catalytic surface. We show the potential of the method by simulating a more complex three-step reaction mechanism with reactant dissociation.

# Gholami | A comparative study of organic solvents in the extraction of lignin and furanics from deep eutectic solvent

Authors Mahsa Gholami, Sascha R.A. Kersten, Boelo Schuur
Affiliation University of Twente

Concerns over negative environmental impact have shifted the attention towards more sustainable alternatives. In this regard, interest in deep eutectic solvents (DES)s as environmental-friendly, low-cost and high-boiling point solvents for biomass delignification is growing.

This work aims to develop a separation scheme to remove lignin and furanics as the main constituents of the stream after delignification using DES made of lactic acid and choline chloride, known as DES-dark liquor. Smink et al showed that lignin dissolved in DES-dark liquor can be recovered by liquid-liquid extraction (LLX) using 2-MTHF. However, lactic acid leaching and solvent cost were found to be hurdles during the separation.

In this study, water precipitation followed by LLX was proposed to limit lactic acid loss in lignin and furanic separation. Furthermore, due to the prior water precipitation, solvent phase properties allow for a wider range of solvents than DES phases without water. Taking this into account, guaiacol is found to be able to replace 2-MTHF. The recovery of lignin and furanics using the proposed process was compared considering 2-MTHF and guaiacol as solvent. The results showed lignin and furanics are recovered with equal recovery ratio using both solvents, while lactic acid leaches less when using guaiacol.

## Graefschepe, van | Low-Temperature Electro-Reduction of Iron Oxide

Authors Niels van Graefschepe, Akmal Irfan Majid, Yali Tang
Affiliation Eindhoven University of Technology

Iron powders are considered to be dense energy carriers which can be combusted to harvest large amounts of heat without any greenhouse gas emissions. The combustion product, iron oxides, can be collected and iron powder can be regenerated using sustainable energy sources to complete the iron fuel cycle. Low-temperature iron oxide electro-reduction could potentially be a suitable iron regeneration method. Although there have been studies in the past which researched the low-temperature electrodeposition of iron, there is a lack of studies which investigate the performance of different low-temperature iron oxide electro-reduction systems and provide a clear comparison between these systems. Therefore, the performance parameters of acidic, alkaline and deep eutectic solvent (DES) low-temperature iron oxide electro-reduction systems, will be experimentally studied in this project.

The main objective of this study is to determine which low-temperature iron oxide electro-reduction systems are suitable for implementation in the iron fuel cycle. Experiments are performed in a parallel plate single electrolysis cell batch setup to study the iron oxide reduction performance in different electrolytes. This performance is studied by analyzing the current efficiency as function of operating parameters such as current density, temperature and iron oxide concentration.

Additionally, the obtained deposits are characterized by visual observation and SEM-EDS analysis. As result, current efficiencies and deposit quality is expected to be influenced by the studied operating parameters. This study is expected to contribute to the development of iron powder regeneration.

# Haven | Light paraffin dehydrogenation using catalyst-functionalized, 3D-printed dense ceramic membranes

Authors Ir. Jord Peter Haven, Dr. Jimmy Alexander Faria Albanese, Prof.dr.ir. Leon Lefferts
Affiliation University of Twente

Non-oxidative dehydrogenation of light paraffins, like ethane and propane, is industrially operated using Pt-based catalysts. This yields high-value olefins (e.g. ethylene, propylene), which are widely used for the production of plastics. The catalyst used in this process consists of Pt supported onto alumina-based materials, because of the high surface area and good hydrothermal stability of these supports. Some of the main drawbacks of the light paraffin dehydrogenation process are: (i) the high temperatures needed due to the endothermic nature of the reaction (e.g. $\Delta H = 137$ kJ/mol for ethane dehydrogenation) and (ii) the thermodynamic equilibrium that limits ethylene formation to ~20% at ~600 °C and 1 bar(a). In order to reduce the energy intensity and to overcome the equilibrium limitation, the produced hydrogen needs to be removed from the reaction zone. This can be achieved by using dense ceramic proton and electron conducting membranes. In this work, the Pt catalyst is deposited directly onto a molybdenum-doped lanthanum tungstate (LWMO) membrane, a promising mixed ionic-electronic conductor (MIEC), to ensure that the dehydrogenation takes place in the immediate vicinity of the membrane. Flat, disk-shaped membranes (D=20 mm) are functionalized, characterized, and catalytically tested in this work. The results provide information on the influence of the support material on the dehydrogenation mechanism and on the location of the dehydrogenation equilibrium. Once this concept is demonstrated we will explore the use of purely proton conducting membranes to electrically drive the hydrogen extraction.

# Hoop, de | Design of Fossil-Free Butadiene Production using Delft Design Map™

Authors Bhatraju, C.; de Hoop, D.; Sultan, H.; Swinkels, P.L.J
Affiliation Delft University of Technology

1,3 butadiene is a major building block in producing synthetic rubbers used in tyre production. Currently, butadiene is produced in a steam cracker which suffers from low and variable yields, leading to supply instabilities and price volatility. An on-purpose production route is needed and an interesting is the production of butadiene from ethanol. In this project, a process for bio-butadiene production is designed using the Delft Design Map™ and integrated with a bio-ethanol plant. The Delft Design Map™ (DDM) is a 12 step design methodology to design a novel process effectively and efficiently. Using DDM, an innovative process is designed that can produce 145 kta of butadiene. The designed process has targeted production of butadiene with an yield of 45 wt%, instead of 5wt% of the conventional route, along with seven technical-grade products that can be readily sold in the market. The production process converts ethanol to butadiene in a one-step process, instead of the traditional two-step process, reducing process complexity. The designed process use carbon-neutral raw materials and utilities which reduces the direct $CO_2$ emissions to zero. The economics and sustainability of the process is improved by taking advantage of the synergistic opportunities between the bio-ethanol and bio-butadiene plants. The mutually beneficial relationship with bioethanol producers resulted in a green premium of 10-20%, competitive to other butadiene from ethanol processes while avoiding 100% of fossil fuels in the production process. The green premium can be further reduced to zero through cost optimisation of raw materials and products.

# Horst | Novel thin-film coatings for next-generation polymer electrolyte fuel cells

Authors Rens Horst, Antoni Forner-Cuenca
Affiliation Eindhoven University of Technology

Recently, research and development of next generation polymer electrolyte fuel cells has intensified as it is viewed as a key technology in the decarbonization of heavy duty transportation (e.g. public transport, land, aviation and maritime freight).[1] However, the current polymer electrolyte fuel cell design suffers from drawbacks that hinder wide-spread commercialization in these sectors. Especially, improved catalyst layers with lower amounts of costly platinum group metals, improved mass transport characteristics at high current densities and increased durability are required. The key is a well-engineered triple phase boundary at the heart of the oxygen reduction reaction in the cathode catalyst layer. At this interface, the electrode microstructure dictates the mass transport of reactant gases and products, while the ionomer film chemistry and morphology define proton availability, but also impact oxygen transport and overall catalyst utilization. A careful balance is required between the transport of reactants, products, protons and electrons. The fabrication of conventional catalyst layer relies mostly on wet chemical synthesis which limits the control over the triple phase boundary microstructure. In particular, poor ionomer distribution was found to impact fuel cell performance negatively.[2] While some catalytic sites are inundated with ionomer and experience a high oxygen transport resistance, other uncoated sites might be starved of protons. Additionally, studies have reported poisoning of the catalyst active sites by adsorption of sulfonic acid moieties present in most commonly used ionomers, which further warrants investigations into alternative ionomer chemistries and coating techniques.[3]

To tackle these challenges, our research will focus on developing novel synthetic methods leveraging electrochemical principles enabling local control of ionomer coating in the catalyst layer. The interest in electrochemical methods originates from their scalability and ability to control the morphology of coatings (e.g. thickness, conformality, porosity and polymer length). At the same time, new ionomer chemistries will be explored and applied using these techniques to impart optimal wettability, ionic conductivity and gas permeability to the materials to enhance electrode performance. The designed materials will be thoroughly characterized and compared against state-of-the-art commercial materials for their performance and durability in a membrane electrode assembly configuration.

**References**

[1] Khedekar, K., Rezaei, M., Besli, M. M., Kuppan, S., Perego, A., Chen, Y., Metzger, M., Stewart, S., Atanassov, P., Tamura, N., Craig, N., Cheng, L., Johnston, C. M., Zenyuk, I. V., Probing Heterogeneous Degradation of Catalyst in PEM Fuel Cells under Realistic Automotive Conditions with Multi-Modal Techniques. Advanced Energy Materials 11, 2101794 (2021).
[2] Ott, S., Orfanidi, A., Schmies, H., Anke, B., Nhan Nong, H., Hübner, J., Gernert, U., Gliech, M., Lerch, M., Strasser, P., Ionomer distribution control in porous carbon-supported catalyst layers for high-power and low Pt-loaded proton exchange membrane fuel cells. Nature Materials 19, 77–85 (2020).
[3] Kongkanand, A., Mathias, M.F., The Priority and Challenge of High-Power Performance of Low-Platinum Proton-Exchange Membrane Fuel Cells. The Journal of Physical Chemistry Letters 7 (7), 1127-1137 (2016).

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# Houben | High pressure $CO_2$-induced plasticization of polymer gas separation membranes

Authors Menno Houben, Romy van Geijn, Joey Kloos, Machiel van Essen, Zandrie Borneman, Kitty Nijmeijer
Affiliation Eindhoven University of Technology

$CO_2$-induced plasticization is a major challenge for polymeric membranes for gas separation. Polymeric membranes lose due to plasticization much of their selectivity, especially at high partial $CO_2$ pressures, resulting in poor membrane performances. Supercritical $CO_2$, $CO_2$ above 31°C and 74bar, is often utilized as an extraction agent in the food industry and in enhanced methane recovery processes. Sc-$CO_2$ has significantly different properties compared to gaseous $CO_2$. The effect of the $CO_2$ fluid properties on the membrane performance and plasticization behavior is not much studied, while it has a large impact in high-pressure applications. Here we investigated the impact of $CO_2$-induced plasticization at high $CO_2$ pressures (up to 120 bar) in polyimide membranes and reflect on the consequences for a $CO_2/CH_4$ separation process.

The transition from gaseous-like to liquid-like sc-$CO_2$ has a major impact on the $CO_2$ density and thus also on the $CO_2$ sorption and permeability. The $CO_2$ permeability increased up to a factor 15 at pressures in the liquid-like sc-$CO_2$ region, which emphasizes the severity of plasticization at these conditions. Plasticization at these high pressures resulted in a huge decrease in membrane selectivity ($CO_2/CH_4$) and thus had a significant impact on the $CH_4$ recovery during a $CO_2/CH_4$ separation process. Calculations showed that the $CH_4$ recovery drops from ~90% at 20 bar to ~28% at 120 bar. This enormously increased CH4 slip at liquid-like conditions not only causes a significant environmental impact, but also affects the economic viability of the separation process.

# Iannizzotto | Tar-free syngas: technological design of a tar cracking unit for B-wood gasification

Authors E. Iannizzotto, S.R.A. Kersten, M.P. Ruiz Ramiro
Affiliation University of Twente

In the present work, the design of a thermochemical tar cracking unit for wood gasification is carried out to meet the requirements of syngas quality for methanol synthesis (<5 mg/Nm$^3$). Tars are produced in a lab-scale bubbling fluidized bed from woody biomass (0,4 kg/h) and fed to a tubular reactor where tar cracking is investigated in the temperature range of 1000-1200 °C varying residence time and reforming agent (steam/air/$O_2$).

The increase of temperature shows a decreasing trend in tar concentration, in favor of higher yield of hydrogen gas and carbon monoxide. Main tar components found in the samples are benzene, naphthalene, anthracene and small quantity of 5-rings PAHs, which appears to be recalcitrant to conversion. Soot is formed as consequence of tar polymerization following the proposed mechanism of HACA addition. In presence of steam, soot is formed in smaller amount.

Higher temperatures and longer residence time (>15 s) are required to reach the required concentration for methanol synthesis. Follow up work will be carried out to find the best operating conditions to reach the concentration target for methanol synthesis.

## Korede | Design and validation of droplet based microfluidic system to study NPLIN

Authors Vikram Korede, Fred Marques Penha, Vincent de Munck, Lotte Stam, Daniel Irimia, Nagaraj Nagalingam, Antoine van der Heijden, Herman Kramer, Burak Eral
Affiliation Delft University of Technology

In an effort to improve our control over crystal size distribution, purity, morphology, and polymorphic outcome, a plethora of methods have been proposed including Non-Photochemical Laser-Induced Nucleation (NPLIN). NPLIN is a physiochemical phenomenon in which a nanosecond laser pulse induces instantaneous crystallization in solutions of low supersaturation which would otherwise take many weeks to nucleate. The term ‘non- photochemical’ implies that the operating wavelength and laser pulse intensity do not induce a photochemical reaction as the solute and the solvent have no absorption bands at the incident wavelength. So far, NPLIN was investigated through irradiating a supersaturated solution in milliliter size vial and later counting the crystallized vials by visual inspection. For each repetition, a new sample vial is manually placed on the beam path, and this procedure is repeated at least 80 to 100 times for statistically accurate measurements. This manual procedure is laborious, time-consuming, and limits the number of experimental conditions studied for the assessment of kinetic parameters. Microfluidics represents an alternative to acquiring automated and statistically reliable data. Thus we design, develop and validate a droplet-based microfluidic platform to quantify the influence of NPLIN on laser-induced nucleation of potassium chloride from solution.

## Leeuw den Bouter, de | On the usage of inline H NMR for the determination of kinetics for $CO_2$ hydrogenation

Authors Prof.dr.ir. J. van der Schaaf; dr. A. Miquelot; dr. P. Oliver, dr, A.Miquelot
Affiliation Eindhoven University of Technology

Nowadays a major search is on the way to develop a method to transform $CO_2$, which is often seen as a waste product due to anthropogenic emissions, into valuable chemicals [1]. One example here is the storage of renewable energy in liquid fuels using hydrogen as an energy carrier [1][2]. Formic acid is often seen as one such a molecule, as it readily allows for a reversible transformation back to hydrogen and $CO_2$ besides being a valuable bulk chemical.

While the reaction towards formic acid has been extensively studied, the nature of the Au active site has not yet been identified. However, based on theoretical studies executed by Lv et al., sub-nanometer gold clusters are likely to significantly contribute to the overall activity. This work aims to synthesize and characterize several supported gold catalysts. Afterwards, their performances for the $CO_2$ hydrogenation to formic acid in terms of activity and selectivity is tested and compared to the commercially available Aurolite catalysts.

The reaction is studied at temperatures between 35-90°C and 10-20 bar using a 1:1 volume mixture of $H_2$ and $CO_2$ in an autoclave, while the employed reduction base is triethylamine. The liquid reaction mixture is continuously monitored using in-line 1H-NMR (Magritek, 43 MHz), thereby allowing for highly efficient screening and kinetic studies. The reliability and optimization of in-line 1H-NMR was verified through comparison with a high resolution 400 MHz off-line 1H-NMR.

[1] A. Álvarez et al., “Challenges in the Greener Production of Formates/Formic Acid, Methanol, and DME by Heterogeneously Catalyzed CO2 Hydrogenation Processes,” Chem. Rev., vol. 117, no. 14, pp. 9804–9838, 2017, doi: 10.1021/acs.chemrev.6b00816.
[2] G. Fachinetti and D. Preti, “PROCESS FOR PREPARING FORMIC ACID,” WO 2012/168396 Al, 2012.

# Maldonado de León | Unveiling the hydrodynamic effects of internal devices in an external-loop gas-lift reactor for syngas fermentation

Authors Héctor Maldonado de León, Lars Puiman, Cristian Picioreanu, Cees Haringa
Affiliation Delft University of Technology

Syngas fermentation is a promising commercial process for converting gaseous streams with a significant CO 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 CO-rich off-gases into ethanol. Recent studies suggest that operating conditions might alleviate typical mass transfer limitations in this process. However, a significant CO-gradient might be observed at large-scale reactors, contributing to performance losses, and imposing some detrimental stress on acetogenic bacteria. A more uniform substrate distribution could prevent these issues.

Adding internal devices for reactor structuring has been proposed to maximize driving forces by modification of flow patterns and interfacial surface in bubble columns and airlift reactors. In the current work, we implemented CFD simulations to unveil the effect of incorporating a degassing unit and perforated plates within the riser of an industrial-scale EL-GLR. Results show that degassing units reduce the presence of dispersed gas in the downcomer up to 25%, thus resulting in an increase of up to 95% of the liquid velocity with respect to a reactor with no internals. Then, the flow resistance upon adding perforated plates can be overcome. Additionally, the presence of perforated plates results in a more uniform gas hold-up along the riser by increasing the residence time of bubbles in each compartment. Thus, the combination of these features contributes to achieving a more uniform substrate distribution in the riser and provides means to select using scale-down studies the environment bacteria will experience within the reactor. Overall, the effect of two types of internal devices was unveiled confirming that each one of them leads towards an improved reactor performance for syngas fermentation.

# Melián-Cabrera | Solvent additive-induced deactivation of heterogeneous catalysts: A case study with Cu on an industrially-relevant hydrogenation

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|---|---|
| Authors | Vanessa Solsona, Silvia Morales-de la Rosa, Oreste De Luca, Harrie Jansma, Bart van der Linden, Petra Rudolf, José M. Campos-Martin, María Emma Borges, Ignacio Melián-Cabrera |
| Affiliation | La Laguna University |

In three-phase reactions, a solvent is used to dilute the produced heat from exothermal reactions. The solvent is usually employed in a large quantity. This means that if it contains an impurity, even at ppm level, the absolute amount can be comparable or higher than the active sites in the employed heterogeneous catalyst. This study reports the effect of low concentrations (ppm level) of a stabilising agent (2,6-di-tert-butyl-4-methylphenol, BHT) contained in an off-the-shelf solvent, on the catalyst performance for the hydrogenolysis of g-butyrolactone over Cu-ZnO-based catalysts. It was found that the CuO-ZnO catalyst performance using a reference solvent (1,4-dioxane) was good, meaning that the equilibrium conversion was achieved in 240 min, whilst a zero conversion was observed when employing tetrahydrofuran. The deactivation was studied in more detail arriving at the preliminary conclusion that the poisoning effect of the solvent´s additive (BHT), present at 250 ppm, inhibits the reaction completely over a CuO-ZnO catalyst. The BHT effect was also extraordinary over a commercial CuO-ZnO-MgO-Al2O3 catalyst but less severe than the CuO-ZnO catalyst; probably due to the higher surface area of the former. The study illustrates the importance of solvent choice and purification for applications such as three-phase catalysed reactions to achieve optimal performance. This work seems to be one of the first studies showing the negative effect of a solvent´s additive on a heterogeneously-catalysed reaction.

This is a joint contribution from TU-Delft, Groningen University, CSIC-Spain and La Laguna University. More Information at Ind. Eng. Chem. Res. 2021, 60, 44, 15999–16010.

# Molder, te | From lignocellulosic biomass to ethylene glycol

Authors T.D.J. te Molder, S.R.A. Kersten, J.P. Lange, M.P. Ruiz
Affiliation Suster BV / University of Twente

Biomass (Biologically sequestered carbon) is besides atmospheric $CO_2$ ¬the only alternative carbon source that could substitute fossil fuels for the manufacturing of chemicals and materials. An interesting case is the production of Ethylene-glycol (EG), a bulk-chemical, is of interest due to the excellent match in elemental composition of biomass feed (saccharide) and glycol products. It was previously shown that cellulose can be selectively converted to glycols via a tungstate catalysed hydrogenolysis route[1]. However, cellulose is typically enclosed in a matrix with lignin and hemi-cellulose and contaminated with inorganic components, proteins and “extractives”.

These fractions could possibly deactivate the catalysts in our system and consequently fail to meet the industrial catalyst consumption window of <1 kgcatalyst/t product [2]. We have developed a flexible hydrogenolysis protocol that is well suited to identify and quantify catalyst poisons present in (lignocellulosic) biomass. We found that lignin retards the hydrogenation function but is not the key inhibitor, as feedstocks high in lignin could still deliver a high EG yield [3]. It appeared that the inorganic components, in particular divalent cations, precipitate the homogenous tungstate catalyst leading to poor glycol yields [4]. These inorganics could be removed by a mild acidic-wash, which allowed glycol yields for woody biomass similar as obtained in a cellulose reference test. However, this mild pretreatment was unsuccessful for grass type biomass which are particular rich in inorganics, proteins and extractives [5]. It turned out that Sulphur, the classical poison, was the root cause for a the poor glycol yield.

References

1. Ji, N., et al., Direct catalytic conversion of cellulose into ethylene glycol using nickel-promoted tungsten carbide catalysts. Angew Chem Int Ed Engl, 2008. 47(44): p. 8510-3.
2. Lange, J.-P., Catalysis for biorefineries – performance criteria for industrial operation. Catalysis Science & Technology, 2016. 6(13): p. 4759-4767.
3. T.D.J. te Molder, et al., Ethylene glycol from lignocellulosic biomass: the impact of lignin on catalytic hydrogenolysis, I.E.C. Research, Editor. 2021.
4. T.D.J. te Molder et al., From Woody Biomass to Ethylene Glycol: Inorganics Removal Boosts the Yield. Industrial & Engineering Chemistry Research, 2021.
5. Submitted to BioPFR as T.D.J. te Molder et al. - Do not forget the classical catalyst poisons: The case of biomass to glycols via catalytic hydrogenolysis

## Nijssen | Lubrication forces in Expanded Bed Adsorption reactors

Authors Tim M.J. Nijssen, Marcel Ottens, Johan T. Padding
Affiliation Delft University of Technology

Expanded Bed Adsorption is a promising biopurification technique, in which unclarified fermentation broth is passed through an expanded adsorption column. The hydrodynamics of the system play a major role in the efficiency of the separation that is achieved. In the poster, we explore the effects of lubrication forces on the bed behaviour and performance.

# Padding | Liquid-Solid Fluidisation: Experimental and numerical insights into heterogeneous liquid-solid behaviour in drinking water softening reactors

Authors Tim Nijssen, Onno Kramer, Peter de Moel, Jamila Rahman, Joppe Kroon, Phoebe Berhanu, Edo Boek, Kay Buist, Jan Peter van der Hoek, Johan Padding, Hans Kuipers
Affiliation Delft University of Technology

Liquid-solid fluidisation is frequently encountered in drinking water treatment processes, for instance in seeded crystallisation softening processes. For modest superficial fluid velocities, liquid-solid fluidisation systems (LSF) are generally considered to be homogeneous, as reported in literature. However, during fluidisation experiments with calcite grains, open spaces of water can be observed between the fluidised particles, even at relatively low fluid velocities. Moreover, significant heterogeneous particle-fluid patterns are detected at higher fluid velocities. Such heterogeneous behaviour can beneficially or adversely affect the chemical crystallisation efficiency. To obtain information about voids in bulk regions, complementary Computational Fluid Dynamics - Discrete Element Method (CFD-DEM) simulations were performed and compared with the experimental results for validation. Simulations were performed using different water inlet velocities and fractionised calcite granules obtained from full-scale reactors. Here, the results are analysed using the bed height, voidage and pressure drop of the system. Furthermore, images of the experiments and simulations are visually compared for the formation of voids. The simulations showed distinct differences in void fraction in the cross-section of the column. It is shown that throughout the range of considered water velocities, heterogeneous behaviour exists and cannot be neglected. The heterogeneity and onset of fluidisation behaviour obtained from the simulations and experimental observations were compared and found to agree reasonably well.

# Pérez-Fortes | Bridging modelling scales in $CO_2$ electrolysis: a solid oxide electrolysis cell case study

Authors Mar Pérez-Fortes, Arata Nakajo
Affiliation Delft University of Technology

Emerging technologies for the electrochemical conversion of $CO_2$ are attracting the attention of the industry and energy sectors aiming at decreasing their carbon emissions. Electrolysers are modular in nature. Their scale-up is however dependent upon the stack (device) design target power density and upon stack integration considerations. Both stem from the technology-developer objectives. Besides each particular company decision and stack size, a $CO_2$ electrolysis plants' size depends upon the market under which it will compete. However, the ultimate decision about the implementation scale must be made concerning also the performance of the whole process together (i.e. pre-treatment, electrolyser, and downstream cleaning units). Therefore, in the ex-ante evaluation and conceptual design of such a process, an appropriate level of modelling detail is crucial to avoid errors and misconceptions arising from extrapolating experimental data at the laboratory scale and/or operation regimes outside from the calibration conditions.

The current work investigates how the $CO_2$ electrochemical reduction to CO behaves when the feed off-gas is recycled, mimicking a plant recycle. It relies on a dynamic modular solid oxide fuel cell model with “1-D + 1-D” spatial discretisation adapted to co-electrolysis. The model is based on physical principles with full coherence in terms of mass transport. Electrode models with distributed charge transport and transfer and dusty-gas diffusion formalism are implemented to capture concentration effects along the stack and through the electrodes. The objective is to identify optimal operating conditions for the stack performance and lifetime and predict possible go/no go plant configurations.

# Polat | Selective Formate Separation Using Redox-Active Polyvinyl Ferrocene-Functionalized Electrodes

Authors Sevgi Polat, Ruud Kortlever, H. Burak Eral
Affiliation Delft University of Technology

Electrochemical separation of formate, a type of organic ion and the smallest carboxylate, has been heavily investigated because the separation challenges in the recovery of carboxylate products formed during electroreduction of $CO_2$ and the purification of water, and in the current chemical and pharmaceutical industries. The objective of the present study was to use a response surface method involving the Box–Behnken design to investigate the fabrication process of polyvinyl ferrocene (PVF) / carbon nanotube (CNT) based electrodes for formate separation and to optimize these electrodes for a higher separation efficiency. First, the fabricated electrodes were characterized using cyclic voltammetry, X-ray diffraction, Raman spectroscopy, and scanning electron microscopy to determine their electrochemical, structural, and morphological properties. Then, Box–Behnken design with a selection of three effective independent variables was applied to determine the optimal conditions for the production of PVF/CNT electrodes with the maximum formate adsorption efficiency. Second-order polynomial equations were developed for the PVF/CNT ratio, sonication time, and ultrasonic amplitude to correlate the parameters. The statistical significance of the model and factors were evaluated using analysis of variance at a 95% confidence level. The optimization results showed that ultrasonic amplitude was the most effective parameter in comparison with other variables and operating at high ultrasonic amplitude and prolonged sonication duration negatively affected formate adsorption efficiency.

# Poto | Techno-economic assessment of the direct synthesis of dimethyl ether via $CO_2$ hydrogenation in membrane reactors

Authors Serena Poto, Thomas Vink, Fausto Gallucci, M. Fernanda Neira d'Angelo
Affiliation Eindhoven University of Technology

Nowadays, dimethyl ether (DME) is produced from fossil fuels (i.e., natural gas), via steam reforming. The benchmark process is energy intensive, with a high $CO_2$ footprint (c.a. 89-98 $gCO_2$/MJDME). Therefore, the use of captured $CO_2$ and green $H_2$ as feedstock for the DME production results as a promising alternative to the conventional route, in view of $CO_2$ valorization. However, this process suffers from strong thermodynamic limitations, especially due to the large volume of water produced. As a result, a significant improvement can be achieved via the in situ removal of water from the reaction environment, by means of membrane reactor.

In this work, we designed and optimized two processes for the one-step $CO_2$ conversion to DME at relatively large scale (i.e., 10 kton/y of DME: 1) a conventional process, based on the packed bed reactor technology (PBR) and 2) an intensified process, assisted by the membrane reactor technology (PBMR). The two processes were first compared on a technical basis: a DME yield of 84.2% and 97.2% is achieved in the conventional and intensified process, respectively. The DME selectivity improved remarkably from 85.7 to 98.4%. An economic analysis was carried out to determine the minimum DME selling price (MDSP), which was found to be c.a. 4 times larger than the current market price. Therefore, we carried out a forecast analysis, to identify scenarios which in the future could make our process competitive with the benchmark. We found that a decrease in the $H_2$ production price from SOEC and a minimum carbon tax of 118 €/ton$CO_2$, would make our technology competitive with the benchmark before 2050.

# Raad, de | The effect of the deployment sequence on the combined $CO_2$ reduction potential of mitigation measures

Authors Brendon de Raad, Marit van Lieshout, Andrea Ramirez Ramirez, Lydia Stougie
Affiliation Delft University of Technology

Continuous retrofits in the industrial sector are needed to meet the set $CO_2$ reduction goals. This study explored the effect of sequencing energy related $CO_2$ mitigation measures on their combined $CO_2$ reduction potential. In a case study of a biodiesel production process, $CO_2$ mitigation measures are deployed in the reaction, separation, heat recovery and power section. The deployment of a membrane reactor, divided wall column, heat pump and an e-boiler in these sections in several sequences showed that the combined $CO_2$ reduction potential is indeed dependent on the deployment sequence. Moreso, the results of the case study demonstrated that the deployment of a heat pump after a divided wall column was technically impossible, but that the combined deployment of a divided wall column and a membrane reactor generated a new heat pump potential. All measures combined in this sequence resulted in the largest $CO_2$ reduction. Though, a different heat pump from the reference case was required, which had its $CO_2$ reduction potential reduced by 50 %. The results of the case study therefore show that using conservative estimates does not provide a proper basis for the combined assessment of $CO_2$ mitigation measures when heat integration measures are considered. Hence, deployment pathways suggested by approaches like the Marginal Abatement Cost Curve, that are based on the stand-alone potential of measures, are likely to give erroneous estimates of the combined potential when heat integration measures are considered.

## Rademaker | Fast, Smart and $CO_2$ free heating in the process industry

Authors Vincent Goovaerts, Kendra Rademaker
Affiliation MEAM BV

Microwave technology has advanced significantly for processing in industrial areas since the 1960's. MEAM is using at least 2cd generation technology for drying and heating purposes.
Here, we would like to present the drying of new types of proteins for use in food and feed. We show that on large scale industrial testing – 500 kg of material – we can achieve significantly shorter drying times compared to traditional techniques whilst also producing a high value product.

## Sajeev Kumar | Integration of Electrochemical $CO_2$ Reduction Reactor into a Process System

Authors Asvin Sajeev Kumar, Isabell Bagemihl, Ruud Kortlever, Ruud van Ommen, Wiebren de Jong
Affiliation Delft University of Technology

The continuous increase in the level of $CO_2$ in the atmosphere and the need to develop an alternate source of energy have steered researchers to explore several mitigation measures such as $CO_2$ capture, $CO_2$ storage and $CO_2$ conversion. Among the various proposed $CO_2$ conversion technologies, the electrochemical $CO_2$ reduction (ECR) is considered to be promising owing to its operational convenience and the possibility to store renewable energy, such as wind and solar, in the form of chemical bonds. Chemical industries and power plants contribute to a major fraction of the anthropogenic $CO_2$ emissions, and would be an ideal source of $CO_2$ for the ECR process. However, one of the major drawbacks is the presence of impurities such as $SO_2$, $NO_2$, $H_2S$, COS and other volatile organic compounds in these sources, which could corrode the system or poison the electrocatalyst. The deactivation of catalyst can also occur due to the presence of trace amounts of heavy metal contaminants such as Fe2+ and Zn2+ in the liquid electrolyte. Hence, this project will focus on the impact of contaminants present in industry-supplied gas streams as well as the liquid electrolyte on the solvent stability and reactor performance. A cleaning criteria will be derived based on these impurity studies, which will be modelled and integrated with the $CO_2$ electrolyser and downstream product separation processes using tools such as Aspen Plus and MATLAB, for the scale-up and techno-economic optimisation of the $CO_2$ electroreduction process.

# Schagen, van | Dynamic modelling of a natural convection-based methanol reactor

Authors T.N. van Schagen, D.W.F. Brilman
Affiliation University of Twente

With the increasing public awareness for climate change and the climate goals set out by the IPCC in mind, carbon capture and utilization is becoming more and more important. One of the ways to utilize the captured $CO_2$ is to produce methanol using sustainable hydrogen. This methanol can then be used as resource in the chemical industry or as a chemical energy storage medium. Bos et. al. [1] developed the Liquid-Out, Gas-In Concept (LOGIC) reactor for producing methanol from $CO_2$ and hydrogen in a highly integrated, intensified manner with a near-100% yield. The reactor integrates a catalyst bed, a heat integration zone and a methanol/water condenser in a single vessel.

The present work focuses on scaling up this reactor, focusing on four points: gas circulation by natural convection, autothermal operation, scalability and intermittent operation. To this end, a one-dimensional dynamic model was developed including natural convection, chemical reactions and heat transfer inside the reactor. First, the different parts (thermodynamics, natural convection and kinetics) of the model were validated individually against experimental results. Second, sensitivity analyses were done on several key design and operating parameters (such as reactor geometry, pressure, temperatures), showing under which conditions the reactor can operate stable and autothermally. The gas recycle rate, pressure and catalyst bed inlet temperature were identified as key parameters for the reactor operation. Third, the startup behaviour was analysed. Finally, the process control strategy for the reactor was developed and tested using the dynamic model.

[1] M.J. Bos, D.W.F. Brilman, A novel condensation reactor for efficient $CO_2$ to methanol conversion for storage of renewable electric energy, Chem. Eng. J. 278 (2015) 527–532. https://doi.org/10.1016/j.cej.2014.10.059.

## Schweidtmann | Process Intelligence Research

Author Artur M. Schweidtmann
Affiliation Delft University of Technology

The transformation of the chemical industry to renewable energy and feedstock supply requires new paradigms for the design of flexible plants, (bio)-catalysts, and functional materials. Recent breakthroughs in Artificial Intelligence (AI) and automation provide unique opportunities for this paradigm change, but only joint interdisciplinary research will unfold the full potential of AI in chemical engineering.

In 2021, we established a new research group at TU Delft that is focusing on AI in chemical engineering. We bridge chemical engineering and AI to deliver the next generation of intelligent knowledge and decision-making platforms for the chemical engineering field. At the heart of the successful transformation of chemical engineering with AI lays our fundamental and applied research in machine learning, data science, and process systems engineering. To bring our vision to life, we are collaborating with industry and academic partners.

## Silva | Chromatographic process development miniaturization: fast results with minimal costs

Authors Tiago Castanheira Silva, Michel Eppink, Marcel Ottens
Affiliation Delft University of Technology

Biopharmaceutical processes heavily rely on chromatographic steps for the purification of their products due to its specificity and better performance than its counterparts. To achieve optimized chromatographic processes, several parameters need to be estimated together with a thorough characterization of protein adsorption behavior, obtained from protein adsorption isotherms. The characterization of different resin-protein pairs and process conditions requires the use of large amounts of materials and samples. High-Throughput Screening has aimed at reducing the costs for process development and optimization, targeting a reduction of material and sample consumption as well as faster assays. This allows to save time and money especially in the early stages of process development.

The most prominent technologies used are liquid-handling stations and microfluidics, the first offering very high automation levels whilst the latter offers very high miniaturization levels. Liquid-handling stations capitalize on the high degree of automation achieved by the equipment which minimizes handling errors. Microfluidics minimizes material and sample consumption, usually in the microliter to nanoliter scale. These two technologies represent different alternatives for process development, enabling fast process development at very low sample consumption.

This work presents a novel microfluidic chip design for the determination of protein adsorption isotherms in batch uptake mode. The microchip allows for a 100-fold decrease in the amount of resin used, compared to liquid-handling stations. The data generated with the microfluidic device is compared to the data obtained using the liquid-handling station, to compare operation and implementation of both technologies.

# Uslu | Furfural valorisation using structured catalysts

Authors A. Uslu, E. A. J. F. Peters, J. A. M. Kuipers and M.F. Neira d'Angelo
Affiliation Eindhoven University of Technology

The increasing scarcity of fossil fuels change has pushed both researchers and the chemical industry to look for alternative feedstocks for specialty chemicals. Lignocellulosic biomass is one of the most interesting feedstocks for this purpose, as it is abundantly available in nature and can be utilized in a wide variety of green bio-based products [1], [2]. This work aims to study the intensification of furfural conversion by studying the application of novel washcoated open-cell metallic foam catalyst in a packed bed reactor.

Open-cell metallic foams consist of interconnected webs of solid material with a large voids between the solid ligaments. The solid structure provides a high surface area while the large voids provides for enhanced hydrodynamic mixing. These characteristics mean that foams are well suited to study the combined effect of phenomena such as mass and heat transfer in catalytic conversions. The aim of this project is elucidating the transport phenomena and chemical behavior governing the conversion of furfural by taking advantage of the increased catalytic and hydrodynamic control provided by foam catalysts [3].

In this work we investigate the application of washcoated open-cell metallic foam catalyst for the conversion of biomass derived furfural. We have developed a coating method that results in a mechanically stable and catalytically active washcoat layer, consisting of $Pd/\gamma\text{-}Al_2O_3$ and $Pd/TiO_2$ on metallic aluminum foams. The catalytically active foam was used to convert biomass derived furfural to the value added compound furfural alcohol at high selectivity.

[1] T. Guo, X. Li, X. Liu, Y. Guo, and Y. Wang, "Catalytic Transformation of Lignocellulosic Biomass into Arenes, 5-Hydroxymethylfurfural, and Furfural," *ChemSusChem*, vol. 11, no. 16, pp. 2758–2765, Aug. 2018

[2] K. Yan, G. Wu, T. Lafleur, and C. Jarvis, "Production, properties and catalytic hydrogenation of furfural to fuel additives and value-added chemicals," *Renewable and Sustainable Energy Reviews*, vol. 38. Elsevier Ltd, pp. 663–676, 2014.

[3] A. Aguirre, V. Chandra, E. A. J. F. Peters, J. A. M. Kuipers, and M. F. Neira D'Angelo, "Open-cell foams as catalysts support: A systematic analysis of the mass transfer limitations," *Chemical Engineering Journal*, vol. 393, Aug. 2020

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# Wal, van der | Optimizing flocculation of digestate to increase circularity in the nutrient recovery from manure

Authors Marrit van der Wal, Kitty Nijmeijer en Zandrie Borneman
Affiliation Eindhoven University of Technology

The agricultural sector aims for valorization of pig manure into separate nutrient-rich fractions for precision fertilization while limiting nitrogen and (climate driven) $CO_2$ emissions. This valorization often involves the production of biogas by co digestion of manure, followed by separation of the solid and the liquid fraction of manure. The organic solid fraction, containing a large fraction of the phosphor, is retrieved as solid fertilizer by mechanical separation, a process often generally improved by the addition of clarifying agents. The liquid fraction is then cleaned of floating parts, after which a high quality liquid stream is obtained that is suitable to be treated by reverse osmosis to produce mineral concentrate and/or nitrogen or potassium rich fractions for precision fertilization [1]. Currently, the dosage of clarifying agent in the solid-liquid separation step is still done rather intuitively which can lead to an overdosage, increasing the operation costs and risk fouling of the RO membranes.

In this study we aim for gaining a better understanding of the flocculation/coagulation mechanism and to improve the solid-liquid separation efficiency by investigating various synthetic polymeric clarifying agents and the addition of iron salt as coagulant. The organic matter removal from the digestate was measured in terms of turbidity and compared to the corresponding dosage of polymer per gram dry matter present in the digestate. Results show that the removal efficiency and its stability depend on the characteristics of the clarifying agents like molecular weight, structure and charge.

[1] Velthof, G.L. (2015) Alterra Report 2650.

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# Weel, ter | Anion exchange membranes for the electrochemical reduction of $CO_2$

Authors Woutje ter Weel, Menno Houben, Zandrie Borneman, Kitty Nijmeijer
Affiliation Eindhoven University of Technology

The electrochemical reduction of residual $CO_2$ towards fuels and chemicals (e.g. ethanol and ethylene) is a promising route to lower our carbon footprint, especially when combined with renewable energy to drive the reactions. $CO_2$ reduction is mainly performed in membrane-containing reactors consisting of an anode and cathode on opposite sides of an ion exchange membrane submerged in an alkaline electrolyte solution. 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 positively charged exchange groups allow for the transport of hydroxide ions from the cathode to the anode. Their main drawback lies in the poor chemical and mechanical stability at high pH and cross-over of negatively charged reaction intermediates.

While extensive research has been performed on electrodes for $CO_2$ reduction, it is yet unclear how the membrane affects this process and what type of membrane would be ideal. Therefore, we focused on commercially available membranes and analyzed their performance in terms of resistance, permselectivity, water uptake, and chemical stability to use as a benchmark for further research. We aim to expand on the current membrane technology by incorporating inorganic additives to improve the mechanical strength and selectivity of the membrane while not compromising the ion exchange capacity. By using wire-based electrospinning a more homogeneous distribution between the organic polymer and inorganic additive is achieved, leading to better mechanical strength and higher ion conductivity in the membrane compared to traditional casting methods.

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# Weijers | Membrane development to make the $CO_2$ plasmolysis more efficient

Authors Cees Weijers, Zandrie Borneman, Kitty Nijmeijer
Affiliation Eindhoven University of Technology

Electrically driven high-temperature electrolysis of $CO_2$ into CO and $O_2$, using solid oxide cells, and plasmolysis are promising routes to reduce the $CO_2$ concentration in air and flue-gases. The produced CO can be upgraded chemical building blocks and to fuel (Power-2-Gas). To increase the conversion efficiency, unreacted $CO_2$ is separated from the dissociated products and returned to the reactor using polymeric hollow fiber membranes.

Asymmetrically skinned hollow fiber membranes for gas separation, were prepared using a dry-wet spinning process and evaluated for use in a Power-2-Gas pilot setup. The membranes, based on a polyimide (Matrimid®), consist of a porous support layer and an ultra-thin dense selective layer on the outside. The thickness of this ultra-thin dense layer can be tailored by controlling the solvent evaporation during the spinning process, which is enhanced by the addition of the volatile co-solvent, acetone, to the dope solution. The nascent fiber first passed through a chimney with nitrogen gas flow to control the evaporation of acetone. This formed a polymer rich boundary layer at the fibers' outer surface. The nascent fiber then entered a water containing coagulation bath, and the polymer rich layer was transformed into an ultra-thin dense selective layer, with a porous supporting layer underneath. Reducing the thickness of the ultra-thin dense selective layer, improves the gas permeation properties. Thicknesses in range of 300-500 nm were achieved by controlling the acetone evaporation, by varying the residence time and the nitrogen flow inside the chimney.

Next, the gas separation performance of the asymmetrically skinned hollow fiber membranes was evaluated (35°C at 4 bar, single gas). For safety reasons, the gas pair $CO_2$/CO has been replaced by CO2/N2 which has comparable permeation properties. Since ultra-thin dense selective layers are especially affected by physical aging, the gas separation performance was monitored over a period of up to 500 days after production.

The results show that physical aging plays a very important role in evaluating the gas separation performance of fresh unconditioned membranes. From these membranes the gas permeation decreases from 21.6 to 2.2 GPU for $CO_2$ and the ideal selectivity from 31 to 22. The values measured after physical aging, can be used to design gas separation modules for the Power-2-Gas pilot setup.

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# Wiltink | Multiscale modelling of $CO_2$ electrochemical conversion- A supply chain perspective

Authors Thijmen Wiltink, Josephine Vos, Andrea Ramirez, Mar Pérez-Fortes
Affiliation Delft University of Technology

To tackle the rising global energy demand and climate change challenge, actions are necessary to reduce anthropogenic $CO_2$ emissions drastically. Utilizing $CO_2$ as feedstock for the chemical industry in an electrochemical process can potentially decrease fossil fuel consumption. In this process, renewable electricity is used to synthesize value-added fuels, chemicals, or products. Currently, the electrochemical reduction of carbon dioxide ($CO_2$ER) is a technology at a low Technology Readiness Level (TRL, between 3-5). The successful deployment of $CO_2$ER will depend not only on the further development and scaling of the technology but also on finding its appropriate role and fitting scale in the near future, among other possible decarbonization options. Sustainability (from a social, environmental, and economic perspective) is crucial for successfully implementing this technology on an industrial scale.

The current project aims to produce essential knowledge on the sustainable implementation of $CO_2$ electrochemical processes under different scenarios. Process Systems Engineering (PSE) and Operations Research (OR) methods and tools are used to evaluate the technology and support the decision-making process in the project. The assessment uses multiscale modeling and optimization techniques at several system levels; the electrolyzer (unit level, reaction pathways), plant (process level, scheduling and operation, plant layouts), and supply chain (system level, optimization under deterministic conditions) levels. The project will propose optimum $CO_2$ER-based plant layouts and supply chains under different scenarios to understand the possible disruptive impact of $CO_2$ electrochemical conversion implementation.

Keywords: $CO_2$ electrochemical reduction; $CO_2$ utilization; multiscale modeling; sustainable design

# Wu | Enhancement of fluidization of cohesive Powders

Authors Kaiqiao Wu, Gabrie M.H. Meesters, J. Ruud van Ommen
Affiliation Delft University of Technology

Gas-solid fluidization is one of the most broadly used techniques in the industry, where homogenous mixing and vigorous interphase contact are of the primary interest. Fine powders (from nanos to a few microns) of a large surface area are typically good candidates for catalytic materials, but their fluidization is problematic, very hard to achieve. At this scale, interparticle forces, such as capillary force and van der Waals force, play a significant role, making the powders cohesive. As a result, an assembly of fine powders tends to agglomerate and creates gas channels when fluidized at a steady flow, leading to rather poor contacts with the supplied gas. Mitigating agglomeration and breaking up gas channels are, obviously, the key steps to improve their fluidization performance. Introducing additional degrees of freedom provides flexibility to manipulate fluidization behavioUr. In the last decade, many works demonstrated the successful uses of external actuators, across different force types and energy sources, to enhance fluidization behaviour.

In this work, we experimentally investigate industrially relevant assistance methods that are prevalent, such as vibration, pulsation. X-ray computational tomography and pressure probes are used to visualize and characterize the hydrodynamics with particular interests to monitor gas channels. By pinpointing the degree-of-enhancement induced and uncovering the underlying mechanism, the results will allow us to optimize existing reactors, and design a new class of efficient production process accordingly.

# Yang | Multi-scale simulation of coke deposition in porous catalytic particles

Authors Xuesong Yang, Shuai Wang, Yurong He, Ivo Roghair, Martin van Sint Annaland
Affiliation Eindhoven University of Technology

Porous catalysts have been widely applied in various chemical processes to increase reaction rates or synthesize specific products. Coke deposition can result in the coverage of active sites and blockage of pores, which lead to catalyst deactivation. The coke deposition inside porous particles is a typical multi-scale process and has different structural features at different scales. In this work, pore-scale and particle-scale simulations are carried out to investigate the characteristics of coke distribution and its effect on heat and mass transfer characteristics. A pore-scale model considering the change of pore structure is established to simulate the coke deposition process in a single pore based on the Lattice Boltzmann method. The results show that the gas rarefaction effect leads to the evolution mechanism of pore structure from the narrowing to the blockage. A particle-resolved model considering the change of physical properties and activity is used to analyze the interaction between transfer characteristics and activity during coke deposition process. In the scope of this work, the dynamic evolution of coke distribution is mainly due to the evolution of pore structure spatial distribution rather than that of activity.

# Zairin | Primary Reactions in Fast Pyrolysis of Plastic Polymers

Authors Dwiputra Muhammad Zairin; Sascha R.A. Kersten; M.P. Ruiz Ramiro
Affiliation University of Twente

Plastic waste accumulation is one of our society's most critical issues, which urges for investigation and development of feasible recycling alternatives. In this context, pyrolysis is one of the most promising approaches to recycle plastic chemically. Plastic pyrolysis has been the subject of much research in the last years; however, the primary reactions of plastic pyrolysis are still known to a lesser extent. In this work, a screen-heater reactor setup was used to investigate the primary reactions of plastic pyrolysis at 400-700 oC. The feedstocks were virgin polymers: polyethylene, polypropylene, and polystyrene. The screen-heater reactor features a fast-heating rate of 2500 oC/s and a liquid nitrogen quick-cooling system, leading to short hot vapor residence times, which allows the study of the primary pyrolysis reactions. The resulting condensable product was analyzed by GC-FID/MS and GPC analysis. The condensable product yield for PE and PP is above 85 %, whereas for PS, it is significantly lower, approximately 50% because most of the styrene monomer goes to the gas phase. Overall, the primary reactions in plastic pyrolysis were found to be random scission of the main polymer chain, which resulted in the formation of shorter hydrocarbons, as well as some end-chain scission to produce monomer in the gas product.

## Zamani Gharaghooshi | Chemical Recycling of Polyurethanes

Authors S. Zamani, J.P. Lange, S.R.A. Kersten, M.P. Ruiz
Affiliation University of Twente

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. Split-phase glycolysis 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-250°C), targeting the production of isocyanates. The products from the reactions have been analysed by LC-UV.

# Zhang | An Edible humidity indicator

Authors Mengmeng Zhang, Abinaya Arunachalam, Kaspar Jansen, Eduardo Mendes, Huseyin Burak Eral
Affiliation Delft University of Technology

We report an edible humidity sensor made up of a protein casein, and a molecular plasticizer glycerol, that mechanically bends upon exposure to humidity. The sensor is a composite material made up of two interfused protein films with varying caseinate and glycerol concentrations. Upon exposure to humidity, each film absorbs different amounts of water and together they bend to report humidity. To rationally engineer the sensor for maximum bending, we characterized the plasticized protein films with microstructure observation as well as thermogravimetric analysis and propose a mechanism relating the glycerol diffusion to the mechanical response. Moreover, we demonstrate that the degree of bending can be tuned by sensor geometry, film thickness and casein/glycerol ratio. We hope that the proposed edible sensor can be placed inside perishable food and pharmaceutical products directly reporting on humidity where it matters, a feat that commercial non-edible electronic and chemo-chromatic sensors cannot provide presently.

# Zhang | Study on turbulent flow and droplets behavior to optimize coalescence filter separators

Authors Weiran Zhang, Ivo Roghair, Martin van Sint Annaland
Affiliation Eindhoven University of Technology

This study will focus on how to optimize the oil-gas separator in the oil-injected screw compressor system. 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) and re-separation (separation of the smaller droplets). In this project, we will focus on how to explore a suitable simulation and experimental approach to optimize separators, including setting a mathematic model to describe the movement, coalescence, and break-up of droplets in separators, designing a new geometry structure of separators, developing a new type of porous filter materials.

# Poster presentations without abstracts

## Bergmans | Solute dispersion in fixed-bed reactors - MRI Tracer Imaging and Pore Network Modeling

| | |
|---|---|
| Authors | Y.E.I. (Yasmine) Bergmans, N. (Noah) Romijn, A. (Ali) Fathiganjehlou, E.A.J.F. (Frank) Peters, K.A. (Kay) Buist, M.W. (Maike) Baltussen and J.A.M. (Hans) Kuipers |
| Affiliation | Eindhoven University of Technology |

## Claassen | Towards modelling of multicomponent transport in large scale particle resolved reactors

| | |
|---|---|
| Authors | C.M.Y. (Claire) Claassen, S. (Samaneh) Tadayon Mousavi, S.M.H.P (Stan) Wintjens, M.W. (Maike) Baltussen, E.A.J.F. (Frank) Peters, J.A.M. (Hans) Kuipers |
| Affiliation | Eindhoven University of Technology |

## Disela | Model-based High Throughput Process Development for vaccine purification - EXPERIMENTAL IMPLEMENTATIONS

| | |
|---|---|
| Authors | Roxana Disela, Daphne Keulen, Geoffroy Geldhof, Olivier le Bussy, Martin Pabst, Marcel Ottens |
| Affiliation | Delft, University of Technology |

## Durubal | Droplet and Catalyst Interactions in Atomization of Bio-Oils

| | |
|---|---|
| Authors | P. M. Durubal, M. W. Baltussen, K. A. Buist, J. A. M. Kuipers |
| Affiliation | Eindhoven University of Technology |

## Eghbalmanesh | The inner life of a packed bed: A DNS approach

| | |
|---|---|
| Authors | A. Eghbalmanesh, M.W. Baltussen, E.A.J.F. Peters, J.A.M. Kuipers |
| Affiliation | Eindhoven University of Technology |

## Elhami | Bio-based crotonic acid from wastewater

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|---|---|
| Authors | Vahideh Elhami, Joao Sousa, Boelo Schuur |
| Affiliation | University of Twente |

## Elisiario | Mass transfer impact on a continuous CO fermentation

| | |
|---|---|
| Authors | Marina P. Elisiario, Floor Schotsman, Henk Noorman, Adrie J. J. Straathof |
| Affiliation | Delft University of Technology |

## Fathiganjehlou | The Inner Life of a Packed Bed: A Pore Network Modelling Approach

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|---|---|
| AuthorsAli Fathiganjehlou, E.A.J.F. Peters, K.A. Buist, J.A.M. Kuipers | |
| Affiliation | Eindhoven University of Technology |

## Gatter | Experimental and numerical investigation of bulk bubble nucleation in supersaturation conditions

| | |
|---|---|
| Authors | Alessandro Battistella, Ivo Roghair, Martin van Sint Annaland, Josefine Gatter |
| Affiliation | Eindhoven University of Technology |

### **Keulen** | Model-based process development for complex vaccine mixtures

| | |
|---|---|
| Authors | Daphne Keulen, Roxana Disela, Geoffroy Geldhof, Olivier Le Bussy, Martin Pabst, Marcel Ottens |
| Affiliation | Delft University of Technology |

### **Leal Perez** | Recovery of carboxylic acids from fermentation broths using reactive extraction and back-extraction: determining the key parameters for optimized downstream processing

| | |
|---|---|
| Authors | Brandon José Leal Pérez, Ioannis Tyraskis, Anu Singh, Marija Saric, Adrie Straathof, Fausto Gallucci, John van der Schaaf |
| Affiliation | Eindhoven University of Technology |

### **Miloshevska** | Flow in fixed-bed reactors: MRI flow imaging and CFD simulations

| | |
|---|---|
| Authors | Marijana Miloshevska, Noah Romijn, Amirhossein Eghbalmanesh, Kay Buist, Frank Peters, Maike Baltussen, Hans Kuipers |
| Affiliation | Eindhoven University of Technology |

### **Nagalingam** | Exploring laser induced thermocavitation for primary nucleation control

| | |
|---|---|
| Authors | Nagaraj Nagalingam, Vikram Korede, Aswin Raghunathan, Daniel Irimia, Remco M. Hartkamp, Johan T. Padding & H. Burak Eral |
| Affiliation | Delft University of Technology |

### **Neijenhuis** | Protein Quantitative Structure Property Relationships for Improved Chromatographic Separation

| | |
|---|---|
| Authors | Tim Neijenhuis, Martin Pabst, Marieke Klijn, and Marcel Ottens |
| Affiliation | Delft University of Technology |

### **Raffel** | Ammonium salt formation during direct fatty amide synthesis

| | |
|---|---|
| Authors | C.M. Raffel, V.P. Sureshkumar, C. Malonda, J. van der Schaaf |
| Affiliation | Eindhoven University of Technology |

### **Rieder** | Prediction of drying profiles of industrial heterogeneous catalysts

| | |
|---|---|
| Authors | D.R. (David) Rieder, E.A.J.F. (Frank) Peters, J.A.M. (Hans) Kuipers |
| Affiliation | Eindhoven University of Technology |

### **Romijn** | The inner life of a packed bed: An MRI approach

| | |
|---|---|
| Authors | N. Romijn, M. W. Baltussen, K. A. Buist and J. A. M. Kuipers |
| Affiliation | Eindhoven University of Technology |

### **Sande, van der** | Gas-fraction distribution measurements in horizontal stirred bed reactors by fast X-ray analysis

| | |
|---|---|
| Authors | P.C. van der Sande, A.C. Vogtlander, E.C. Wagner, G.M.H. Meesters, J.R. van Ommen |
| Affiliation | Delft University of Technology |

### **Sureshkumar** | Nitrile hydrogenation on structured foam catalysts

| | |
|---|---|
| Authors | Prof.dr.ir. J. van der Schaaf; dr. M.F.Neira d'Angelo; dr. Co van den Berg |

Affiliation Eindhoven University of Technology

## Varghese | Electrochemical $CO_2$ reduction reaction in a flow cell

Authors Merin Varghese, Dr. Marta Costa Figuereido, prof.dr.ir. J. van der Schaaf
Affiliation Eindhoven University of Technology