# Annual Report 2023



Extruded sodium alginate produced through a slit-die directly from the extruder. Materials prepared by Dr. Arianna Rech.

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## Annual Report 2023

In 2023, DTU secured the top position in the new EngiRank ranking, which assesses the quality of European technical universities in the EU. The evaluation spanned 225 technical universities across 27 countries, considering factors such as citation and patent statistics. Regarding Research, Innovation, Teaching Quality, and Sustainable Development Goals, DTU ranked no. 1 in Chemical Engineering. While we take immense pride in this position, we acknowledge the strengths of our many partners throughout Europe, and fostering partnerships with other universities remains a high priority for our department.

This year's annual report highlights a spectrum of great research projects in our field of chemical and biochemical engineering covering product design, process design, and production across chemistry, biotechnology, food, pharma, and energy. How food waste can be used for a range of products, from biogas that can replace fossil fuel to biopolymers that can replace oil-based plastic. How a collaboration between DTU Chemical Engineering, ROCKWOOL, and FLSmidth leads to lower climatic impact from the manufacturing of building materials and how we improve both the functionality and sustainability of intumescent coatings, making fire protection both better and greener at The Hempel Foundation Coatings Science and Technology Centre (CoaST).

DTU Chemical and Biochemical Engineering is proud to host three recipients of the prestigious European Research Council Advanced Grant. In 2023, Irini Angelidaki received her grant, enabling research in a completely new way of conducting fermentations with designed microbial consortia, further strengthening the green transition. In this report, our second ERC recipient, Professor John Woodley, revisits the roots of chemical engineering and our third recipient, Professor Georgios M. Kontogeorgis contributes to a research project into the surprisingly anomalous properties of water.

Education is the most important outcome of our department. We launched a new industrial MSc education in Biomanufacturing in 2023. The students are employed at one of the Biotech City Kalundborg companies while studying, ensuring practical experience and an almost certain job guarantee after graduating. Along with the partners of Biotech City Kalundborg, we aim to educate up to 40 students per year.

Looking ahead, we will update the 2021 digitalization strategy that has established us as a department that takes leadership in digitalization for the chemical and biochemical domain both internally at DTU and externally in cooperation with the private sector and internationally through focused dissemination of our activities. Until now we have largely focused on our pilot plant but will gradually expand to include research exploring AI and machine learning, quantum computing, and quantum AI as well as digital tools and AI in education. They are all essential to sustain the department's ability to offer education and scientific solutions for the future.

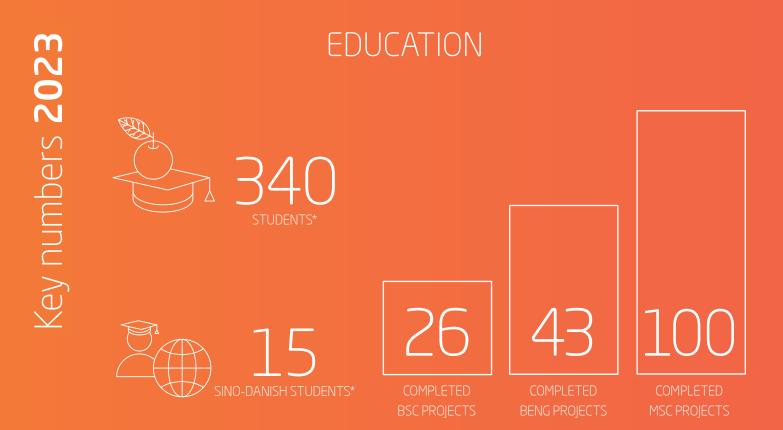
We remain committed to staying at the forefront knowing that excellence requires hard work through cooperation with industrial and academic partners. Our accomplished employees play a pivotal role in upholding this commitment, ensuring that we consistently deliver results to support the journey of chemical and biochemical engineering into a still more sustainable future. We invite industrial and academic partners to collaborate, joining us on this journey.

Him Dan John

Kim Dam-Jøhansen Professor, Head of Department



Kim Dam-Johansen Professor, Head of Department



## RESEARCH



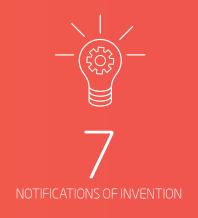
228 SCIENTIFIC ARTICLES IN NOS-INDEXED JOURNALS





\* Based on STÅ. One STÅ is the equivalent of one student studying full time in a yea

## INNOVATION



## ORGANIZATION











32 FACULTY MEMBERS



RESEARCHERS / SENIOR RESEARCHERS



PHD STUDENTS INCLUDING 6 INDUSTRIAL PHD'S



## Biopolymers as replacement of commodity plastics

Alginates and other biological polymers show great potential as future raw materials for plastics.

Soon, biological compounds may replace petrochemical raw materials for polymer production. In nature, materials like alginates, cellulose, and chitosan perform tasks that resemble those of household polymers. According to work in the Danish Polymer Centre (DPC), DTU Chemical and Biochemical Engineering, it is possible that certain biological polymers can substitute fossil feedstocks for specific purposes. "Thereby, biopolymers can contribute to green transition and serve as a renewable source of much needed raw materials," says Associate Professor Anders E. Daugaard, DTU Chemical and Biochemical Engineering. DPC researchers take part in several projects that focus on exploiting biopolymers as sources for new materials. Some projects involve combinations of biopolymers found in nature and biopolymers produced from agricultural waste, food waste etc.

### How biopolymers can become processable

An obvious challenge is the fact that biological polymers are not optimized for industrial processes. This is a major focus of efforts in DPC. A study by PhD student Arianna Rech, DPC, has established how direct processing of biopolymers can be enabled through the formulation of biopolymers, leading to lower temperature processing and preparation of materials that are remarkably similar to the currently known plastics. Through establishing a balance between plasticization and processing aids, the study shows how it is possible to obtain processable biopolymer-based materials.

The approach has been applied to the preparation of fiber-based composites and the preparation of various alginate-based composites.

"Though they are not strictly thermoplastic, with enough water as processing aid, the mixtures become processable by common plastic processing techniques such as extrusion and 3D printing," explains Anders E. Daugaard.

The research has been conducted in close cooperation with the Center for Information

Technology and Architecture (CITA) at the Royal Danish Academy as well as through several industrial research projects.

### Alginates are flexible as raw materials

By use of permanent plasticizers such as polyols - e.g., glycerol - it is similarly possible to tailor the final properties of the processed materials and prepare materials that are comparable to commonly known plastics.

"Particularly alginates are an interesting category of materials showing immense potential for a broad selection of applications. Alginates have been shown to be recyclable and can be prepared by mixing with waste materials from food production. This leads to a reduction in consumption of pristine materials and correspondingly to a lower overall sustainability impact of the material," says Anders E. Daugaard.

Alginates have thus been established as a good platform for replacement of simple forms of plastic.

Through a variety of recently initiated projects, DPC will continue to explore production and application of biopolymer-based materials.

Associate Professor Anders E. Daugaard

## Third-generation biopolymers

Today, most plastics originate from petrochemical raw materials. In the interest of green transition, there is a need to reduce the impact of plastic production by finding more sustainable raw materials.

The earliest biopolymers were produced from agricultural products such as sugar, corn, and potato starch. These first-generation biopolymers have the obvious drawback of having to compete with food and animal feed industries for raw materials. Thus, attention soon shifted towards secondgeneration biopolymers that are produced from agricultural waste products, household waste, and waste from the food industry.

Recently, algae and other fast-growing species, currently not used extensively for nutritional purposes, have come to attention as feedstock for polymer production. This is known as third-generation biopolymers.

## The Danish Polymer Centre

The Danish Polymer Centre aims at being at the forefront of the synthesis and characterization of novel polymer materials with a special emphasis on silicone polymers and sustainable polymers. Currently, most focus is directed towards sustainable polymers, plastics, and elastomers for use in a variety of applications, such as commodity plastics, advanced electronics, and soft robotics.

The main objective of the research area is to lead the way toward more sustainable materials. We aim to take part in the transition at all levels of materials development from the fundamental synthesis of new bio-based polymers, across various recycling pathways and toward industrial implementation.

In society, we are targeting a more sustainable use of all materials and plastics in particular. There are a number of pathways towards reaching this – both from a materials sourcing point of view, as well as through conservation of the materials we have and using them in the best possible way. In our efforts to contribute to this challenge in society, we collaborate across the relevant disciplines to take part in the development of the new systems that we require as tomorrow's materials.

Specifically, we currently have research activities in the areas of greener production, using both enzymes as well as classical synthetic methods to prepare polymers from new sources of raw materials. By exploiting waste materials or bio-based raw materials, we target the preparation of materials with a lower impact. Through collaborations, we exploit both chemical, biological, and mechanical recycling to prepare new products or materials that enable easier recycling and permit either simpler or direct recycling of materials. This also encompasses the synthesis of additive components to enable systems to be recycled directly and to simplify these systems to increase their value in a circular economy context. These activities are supported through our strong chemical synthetic and characterization platform, which we exploit across a broad range of products both in collaboration with other academic institutions as well as with industry.

## Less CO<sub>2</sub> from production of building materials

A collaboration project with ROCKWOOL, FLSmidth and DTU as partners leads to lower climatic impact from the manufacturing of buildings materials.

Through a series of chemical engineeringbased improvements, it is possible to achieve significant reductions in the carbon footprint from production of materials for the construction industry. The research and development results have been achieved in a collaboration of ROCKWOOL, FLSmidth and CHEC.

"FLSmidth provides equipment for the cement industry, and ROCKWOOL produces mineralbased isolation materials. While the two companies are not competing, they both use high temperatures processes in their production technology, which have many similarities," says Senior Researcher Peter Arendt Jensen, CHEC.

The project was entitled "Process technology for sustainable Building materials production" – or ProBu for short. Some of the improvements achieved in ProBu enable use of waste materials as fuel, while others are related to higher energy efficiency during manufacturing. The ProBU project was financed by Innovation Fund Denmark through the Grand Solutions Program.

## Enabling increased use of waste as fuel on cement plants

Substituting fossil fuels for waste-based fuels will not only reduce net CO<sub>2</sub> emission but may also improve cement plant economy. However, using waste as fuel does involve various challenges, some of which were addressed in the project. Increasing the amounts of waste-derived fuels at a cement factory will typically increase the amount of chlorine (Cl) and sulphur (S) fed into the cement plant. Presently this is dealt with by making a purge stream of gas from the plant which reduces the levels of Cl, but also reduces the thermal efficiency of the plant, and therefore limits the amount of wastederived fuel that can be applied.

"Based on fundamental studies on the release of Cl and S from cement raw meal a new concept for removing both species from a cement factory was proposed. The technology still needs some development to be commercially available, but it can potentially remove Cl and S simultaneously from the plants, while keeping a high thermal efficiency," explains Associate Professor Hao Wu, CHEC.

## Moving beyond trial-and-error

The ROCKWOOL melting technology has in the later years been further developed to a shift in the applied fuel from coal coke, to pulverized coal, to gas and further to renewable electricity. All the steps have led to a decreased net CO<sub>2</sub> emission per produced isolation material product. The latest development has been to base the melting process on the use of electrical heating.

In both ROCKWOOL and cement plants, preheater cyclones are important components, which are needed for a high energy efficiency of the plants is wanted.



Senior Researcher Sønnik Clausen and Associate Professor Hao Wu in the CHEC pilot hall 👸 Christian O. Carlsson

"However, the detailed flow behavior in such industrial scale cyclones is difficult to predict and thereby design is often done as a trial-and-error experimental development. To improve the understanding of industrial preheater cyclones a CFD model (Computational Fluid Dynamics, ed.) that can account for the two-phase flow, particle separation, particle agglomeration, heat transfer and erosion was developed. The model has been verified by use of full-scale industrial measurements and is now provided to the companies as a tool that can be used for future design and optimization of cyclone preheater systems," explains Hao Wu.

## Geo-polymers as alternative cement

Traditional Portland cement production is responsible for considerable amounts of CO<sub>2</sub> emissions due to both the calcination of limestone and the high temperatures used in rotary kilns (up to 1500°C) required to obtain the cement product. However, alternative cement based on clays, wastes, and strong bases, so called geo-polymers, can obtain similar strength properties while emitting much less CO<sub>2</sub> in the production process. A PhD project on geo-polymer properties and process technologies was conducted and provided valuable data on the possible future use of geo-polymers.

"The geo-polymer-based concrete production still has some challenges to overcome, such as supply chain, infrastructure, costs, and standardization. Nevertheless, this PhD study has provided data that indicates that if prescriptive standards are provided, and more strict CO<sub>2</sub> taxes are enforced, then geo-polymers can be a very relevant alternative to traditional Portland cement," says Peter Arendt Jensen.

With respect to emissions from production processes, most focus has been directed towards minimizing nitrogen oxide (NO<sub>x</sub>) emissions. Previously developed fundamental knowledge on nitrogen chemistry has been applied in CFD modelling to provide an improved understanding of the interaction of flow, combustion, and nitrogen chemistry in industrial reactors. Two examples of high temperature reactors were simulated using CFD models that also account for combustion and NO formation. Examples included the ROCKWOOL melting cyclone and an FLSmidth calciner. The calciner modeling was evaluated by full detailed scale measuring data. The models have provided new insights with respect to the complex mechanism of formation and destruction of NO<sub>x</sub> in industrial reactors.

## Promising innovations in both companies

As part of the project advanced measurements on industrial reactors were conducted both to obtain an improved understanding of the processes and to support the development of mathematical models. The measurements included both probe based and optical measurements, and included data on gas, gas composition, temperature, local deposit formation and video registration of the reactor chamber. A range of reactors e.g. a preheater cyclone, melting cyclone, calciner and electrical heating equipment were investigated.

"A large range of unique data was provided that supported the conducted project activities," says Peter Arendt Jensen, while noting that besides new insights, the ProBu project has resulted in the education of five PhDs, and strengthened collaboration between the companies and DTU: "Several new collaboration projects have been initiated based on the ProBu collaboration." Also included in the project were development activities at the companies. At ROCKWOOL, the Integrated Melting Furnace was converted from coal combustion to run on biogas fuel, and furthermore the first cupola mineral technology has been developed to operate on electrical heating. FLSmidth has developed the FUELFLEX Pyrolyzer technology that leads the way for 100 % waste firing on calciners, and furthermore leads to large reductions in the NO<sub>x</sub> emission from cement plants.

Associate Professor Hao Wu and Senior Researcher Peter Arendt Jensen

## CHEC

The CHEC Research Centre at DTU Chemical Engineering carries out research in fields related to chemical reaction engineering, with the focus on catalysis and on thermal processes such as combustion, gasification and pyrolysis. The aim is to facilitate the transition to more sustainable and cleaner processes in fuel and chemical, heat and power production, transportation, energy-intensive industry and agriculture.

Important areas include Power-to-X technologies, development and application of carbonfree energy carriers such as ammonia or metals, use of sustainable resources such as biomass and waste for production of power, fuels and other products such as biochar, and emission control.

CHEC has achieved international recognition through a combination of experiments and mathematical modeling, based on chemical kinetics, chemical reaction engineering, thermodynamics, and fluid dynamics.

Laboratory reactors are used to characterize gas-phase, gas-solid and catalyzed reactions at atmospheric or high pressure in a wide temperature range, sometimes in combination with IR and X-ray spectroscopy. Extrapolation to industrial scale is conducted by use of pilot-scale experiments or full-scale measuring campaigns, often combined with computational fluid dynamics (CFD).

# Advances in coatings for passive fire protection

The Hempel Foundation Coatings Science and Technology Centre (CoaST) at DTU has become one of the largest research groups within intumescent coatings.



Much like the airbag in a car, the ability of a coating to provide passive fire protection will hopefully never be displayed. But should a fire break out, the best so-called intumescent coatings are able to swell by as much as 100 times into a foam which will quickly stiffen. This layer of char is thermally insulating, meaning that the inevitable heating of the underlaying structure takes place at a significantly reduced pace, which potentially can save lives. Without this protection, a material like for instance steel could quickly loose strength leading to collapse of the structure.

An area of focus at CoaST at DTU Chemical and Biochemical Engineering is to improve not only the functionality of intumescent coatings but also their sustainability. Today, CoaST is one of the largest university-based research groups within intumescent coatings.

"Intumescent coatings offer a high degree of fire protection relative to the use of material. However, further improvements in efficiency and sustainability are possible but innovations must meet other industry requirements such as easy application and maintenance," says Asst. Professor Jochen Dreyer, CoaST.

PhD student Hafeez Ahmadi preparing the CoaST Fire for testing of an intumescent coating. Orte Vestergaard Poulsen Sommer

### Several reactions behind formation of char

A closer look at the involved mechanisms reveals several temperature-activated reactions such as softening, foaming, carbonization, and oxidation to form the char structure. All these areas are covered at CoaST. Recent projects include the development of better and faster testing methods. Special focus is on the influence of the testing conditions, comparing industrial scale gas fired furnaces to lab scale ovens and how the thermal boundary conditions, gas composition, or substrate geometry might influence the test results. The experimental studies are supplemented by CFD (computational fluid dynamics) simulations of the various systems.

CoaST is also working on the detailed characterization of the formed chars, combining fluorescence microscopy with scanning electron microscopy and image processing. "The aim is to better understand how the porosity and pore size distribution influence the insulation properties and how the obtained char morphology is influenced by the testing conditions. These insights will allow manufacture of coatings with a given desired char pore structure," says Jochen Dreyer.

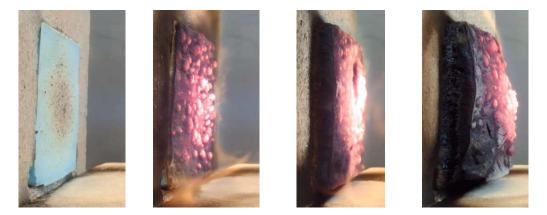
In a related effort, CoaST is working on numerical models to describe the processes taking place during intumescence. Another area at CoaST is intumescent coating formulation. Intumescent coatings are predominantly organic-based leading to major drawbacks including toxic ingredient incorporation, toxic smoke and gas release, and potential low mechanical strength of the expanded char. To combat these limitations, research on ingredient substitution or even alternative intumescent coating concepts is increasing with the aim of providing sustainable and cheap fire protection of construction materials.

## Inorganic alkali silicate coatings display potential

Novel systems with improved health and sustainability profiles are a focus in CoaST, not least inorganic-based coatings. Here, the potential of inorganic alkali silicate coatings and geo-polymers to induce intumescence with the release of only water has been reported. However, these coatings in their pure form exhibit low thermal stability and generally high sensitivity to carbon dioxide and water due to their hygroscopic nature.

Recently, a predominantly inorganic intumescent coating has been developed at CoaST showing superior fire protection potential in lab-scale conditions. Compared to commercial intumescent coatings, it is flame-retardant with release of significantly lower amounts of smoke and toxic gases. Moreover, the expanded coating is of a relatively high structural integrity.

Due to these promising properties, CoaST researchers were granted the opportunity to carry out tests in an industrial furnace at Hempel A/S. Unfortunately, the coating



The intumescence process of an organic-based coating exposed to an impinging flame.

did not expand sufficiently in the industrial furnace, leading to poor fire protection. Differences in scale, geometry, heating source, and chamber environment have been pointed out. These findings emphasize the need for an improved understanding of the various test methods.

PhD Student Hafeez Ahmadi and Asst. Professor Jochen DreyerProfessor Jochen

## CoaST

The Hempel Foundation Coatings Science and Technology Centre

CoaST is a leading centre for research, innovation, and education in sustainable and primarily organic coatings technologies. CoaST covers coating technologies along the entire value chain from raw materials, over formulation, test and characterization to production and application. In the broad perspective, CoaST activities support development, production, and use of coatings with improved sustainability profiles over the lifetime of the coating.

### Coatings for a better future

Coatings are highly complex multicomponent products, which must fulfill many conflicting requirements. Important properties are, for instance, strong adhesion to the substrate or underlying coating layers, adequate viscosity profile, long durability, continuous or durable appealing appearance, and all this at a competitive cost. Functional coatings, in addition, must e.g. provide substrate protection such as resistance against corrosion or biofouling, provide longer escape times during a fire, or remove pollutants through catalytic activity.

Within the area of sustainable coatings science and engineering, CoaST aim to:

- provide in depth knowledge of current coatings challenges
- understand the fundamental working mechanisms of coatings
- develop mathematical tools that quantify coating behaviour
- design and use equipment for accelerated testing of coatings
- design coatings that set new standards with respect to more sustainable formulations and efficient functionalities

Presently, research activities in CoaST focus on the following areas:

- Sustainable raw materials for coatings
- Coating formulation and production principles
- Fouling control coatings
- Anti-corrosive coatings
- Intumescent coatings
- Other functional coatings

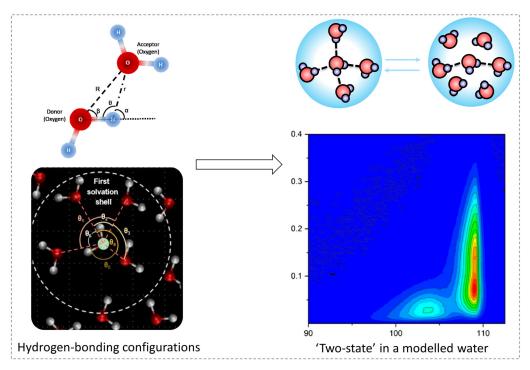
The CoaST research approach is based on classical chemical engineering tools combined with formulation expertise often in close co-operation with industrial partners. CoaST's research covers from basic to applied research and range from laboratory work to model based test programs to natural ageing exposures. CoaST's fundamental coating research supports the traditional more empirical approach of the coatings industry and is focused on improved sustainability profiles.

## Progress in modeling of thermodynamics for water

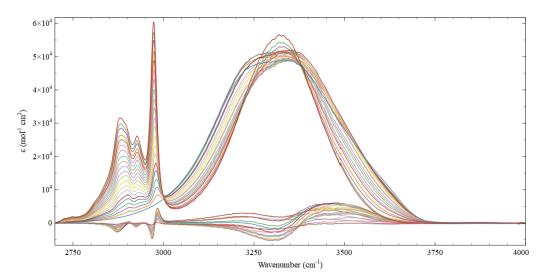
Research at DTU Chemical and Biochemical Engineering suggests that molecular thermodynamics models can satisfactorily represent the anomalous properties of water by integrating different hydrogen-bonding possibilities.

Despite the simplicity of a single water molecule, water is highly complex, possessing a range of properties untypical for a liquid. Until now, even the most advanced thermodynamic models have failed to describe these anomalous phenomena. However, resent progress in applied thermodynamics at DTU Chemical and Biochemical Engineering is about to change the picture. By enabling state-of-the-art molecular theory for associations to accommodate multiple hydrogen-bonding schemes, a model can satisfactorily represent the anomalous properties of water.

Water is the most essential fluid on our planet, and it plays important roles in a wide variety of



The many anomalous properties of water present significant challenges for advanced molecular thermodynamic models, while the 'two-state' theory is gaining significant recognition in explaining the anomalous behavior of water. Molecular dynamics simulations provide an intuitive way to bridge them. This figure shows that molecular dynamics simulations can show two local structures from hydrogen-bonding configurations, which gives inspiration on how to improve the advanced molecular thermodynamic models.



ATR spectra and excess spectra of solutions of water and ethanol with molar fractions varying from 0 to 1 with a step 0.05. The spectra are expressed as extinction coefficients in order to remove optical and density biases

fields. An example of an anomalous property is the fact that water becomes less dense when it enters its solid phase, ice. Water has a density maximum at 4 °C, which makes ice float in water, and this behavior plays an important role in controlling temperature distribution and vertical circulation and increasing the chances of survival of organisms in water. Further, water has a very high heat capacity, which prevents large temperature fluctuations and maintains uniform body temperatures, important for biochemical processes. Water's heat capacity and compressibility present minima as temperature changes.

## Successful introduction of parameter set

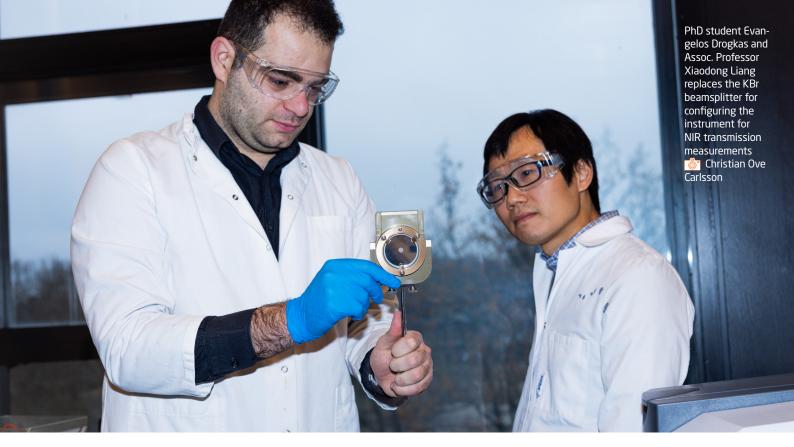
Research on water at the Applied Thermodynamics Center for Energy Resources Engineering Center (AT-CERE) at DTU Chemical and Biochemical Engineering can be traced back to before 2000. At that time, a robust parameter set for modeling the phase behavior of water with the Cubic Plus Association equation of state was developed. Unlike many other models which have many different sets of water parameters from different groups, the parameter set of this model has been kept and successfully used for all important applications over the past 25 years. However, this model - just like other advanced thermodynamic models - failed to describe the anomalous properties of water.

With the award of the ERC (European Research Council) Advanced Grant "New Paradigm in Electrolyte Thermodynamics" to Professor Georgios M. Kontogeorgis, water research at AT-CERE was boosted. Since water is the most important and commonly used solvent in electrolyte solutions, water research was identified as a key element in the research program on electrolyte thermodynamics. Especially two questions were addressed. Firstly, to which extent can the state-of-the-art molecular dynamics represent the anomalous properties of water? And secondly, will a phenomenological two-state theory model suffice?

In the meantime, fundamental research using molecular dynamics simulation, supported by PetroChina, was conducted to investigate the relationship between the structure and properties of water. Here, new methods on how to identify and quantify locally favored tetrahedral structures in different water models were proposed.

### Water as a two-state liquid

These research activities led to the conclusion, that the dynamics of different structures need to be considered in modern molecular thermodynamics models to correctly capture the anomalous properties of water as well as to accurately describe the phase equilibria of water-containing mixtures.



With the award of the Villum Experiment project "Is Water a two-state liquid?" to Professor Georgios M. Kontogeorgis significant further progress is made. According to initial results, with two different hydrogen-bonding possibilities in dynamic equilibrium, the modern molecular thermodynamics models can satisfactorily represent the anomalous properties of water such as density maxima and compressibility minima. The water research at AT-CERE will continue with the aim of developing a general model which can accurately describe water's anomalous thermodynamic properties and predict the phase behavior of water-containing multicomponent and multiphase systems.

Associate Professor Xiaodong Liang and Professor Georgios M. Kontogeorgis

## **Research on water treatment**

Besides the molecular thermodynamics research, several other projects on water are carried out at AT-CERE. In the Villum Experiment project "Testing of a pulsed electro/ magnetic field device on Marine gasoil and water", awarded to Senior Researcher Michael Bache, NMR and IR have been used to study the interaction of water and peptides with chiral groups, aiming to explain the biological activity difference of different chiral peptides. Further, the effects of pulse electro/magnetic/ acoustic treatment of water, resulting in an impact on the CaCO<sub>3</sub> scaling dynamics in drinking water, was/is been studied in three other projects: The Danish Maritime foundation, Lagur A/S project; AMTech Aqua Miljø ApS Kalkknuser undersøgelser KARAKALK VIS project; "Chalk'Gus" Innovationspartnerskab, CLEAN – Danmarks Miljøklynge Innovationskraft Miljøteknologi 2023-2024.

For further details contact Senior Researcher Michael Bache at KT.

## AT CERE - Applied Thermodynamics-Center for Energy Resources Engineering

AT-CERE stands for Applied Thermodynamics – Center for Energy Resources Engineering. The AT CERE Research Centre, as part of DTU's Department of Chemical and Biochemical Engineering, is a centre focused in the areas of Applied Thermodynamics, transport properties and processes, materials science, fermentation technology and mathematical modelling with applications to the energy sector incl. petroleum technology, CO<sub>2</sub> capture, utilization and storage, chemical industry as well as biotechnology with emphasis on biorefinery conversions.

AT CERE is associated with the DTU interdepartmental activity CERE, which is Denmark's leading research centre in a wide range of energy resources which, in addition to the above, also include geoscience. AT CERE and CERE host an industry consortium, which includes around 15 companies from all over the world.

AT-CERE is committed to perform high-quality experimental and theoretical research with international impact, in which we often combine the above disciplines in broader projects of interest to chemical, energy and biochemical engineering. Both fundamental and applied research is being conducted. Many of the applied problems are inspired by or based on input from CERE's industrial consortium.

## **Our History**

AT CERE has, in its various forms, a 30+ years history. The centre in its original form (first as a centre in applied thermodynamics, and later, since 1987, in the form of an engineering research centre, IVC-SEP) was established in the early 1980's by Professor Aage Fredenslund, who was succeeded in the leadership in 1994 by Professor Erling Stenby. Since 2009 AT CERE's activities are connected to DTU's interdepartmental activity CERE.

For more information, please visit CERE's website: www.cere.dtu.dk

### Main deliverables to the Consortium members

Corporate members of the Consortium can access and obtain all results directly from the Center for Energy Resources Engineering as soon as they become available, usually one or two years before publication. A computer program for Separation and Phase Equilibrium Calculations, SPECS, is made available for members of the Consortium. A wide range of other software tools are also available to member companies as well as access to an electrolyte database and other facilities. Consortium members are offered also favourable prices for PhD courses organized by the centre as well as access to experimental facilities. Also, students and scientists from the Center for Energy Resources Engineering are available for collaboration with consortium members on projects conducted at company facilities.

## Upgrading of biogas into high-quality methane

A technology developed at DTU converts biogas efficiently into biomethane. Thereby, biomethane can contribute to the Danish government's strategic target of fossil-free energy supply.

Conversion of biogas into biomethane with a methane content above 98% has been achieved by researchers at DTU Chemical and Biochemical Engineering and partners.

"The resulting product can be used directly in the natural gas grid or for other applications such as Liquid Natural Gas (LNG). Thereby, biomethane can contribute to the Danish government's strategic targets of fossil-free energy supply by 2050 and 55% renewable energy by 2030," says Professor Irini Angelidaki, DTU Chemical and Biochemical Engineering.

Over the latest decades, biogas production has become a significant part of the energy sector in Denmark and some other European countries. Biogas is produced by anaerobic digestion by microorganisms of manures, industrial food waste, and other organic residues.

### Upgrading increases the value of biogas

Biogas consists mainly of methane (approximately 60%) and  $CO_2$  (approximately 40%). Since the  $CO_2$  content prevents direct substitution of natural gas, the biogas has typically been used for production of electricity and heat by combustion in gas motors.

However, other renewable energy technologies such as wind turbines and photovoltaics have become better options for production of electricity and heat. Biogas should instead be reserved for higher value purposes. This requires removal of  $CO_2$  from the biogas. The field is known as biogas upgrading.

Researchers at DTU Chemical and Biochemical Engineering have been working on biogas upgrading for many years. The new concept for conversion of biogas into high-quality methane is developed by the Bioconversions group (or Biocon for short) as part of the eFuel project funded by the Danish Energy Agency. Industrial partners in eFuel are Nature Energy and Biogas Clean, while DTU and the University of Southern Denmark (SDU) are academic partners.

### Microbes are immobilized

Around 40% of the methane consumption in Denmark is upgraded biogas. The current upgrading methods include water scrubbers, membranes, and amines. These technologies have adverse effects such as methane emission or addition of chemicals. Further, these methods do not capture CO<sub>2</sub> from the biogas but emit the CO<sub>2</sub> into the atmosphere.

In the new process, the  $CO_2$  in biogas is converted into methane in a biological process catalyzed by anaerobic methanogenic microorganisms. In this reaction hydrogen (H<sub>2</sub>) produced from water electrolysis (Power-to-X) using residual electricity is reacting with CO<sub>2</sub> in biogas to produce biomethane. The researchers have constructed an efficient process in a trickle bed reactor (TBR). "The microbes can be immobilized on the packing material which should have a high surface-area for gas-liquid mass transfer favoring the high density and activity of methanogenic archaea. Also important is good contact between the gases (H<sub>2</sub> and biogas) and the microorganisms," explains Irini Angelidaki.

## **Enrichment of specific bacteria**

During the pilot trials, the TBR was fed with real biogas as CO<sub>2</sub> source under progressively increased gas provision rates. Additionally, genome-centric metagenomic analysis was applied to gain insight into the microbiome of the reactor.

A maximum methane content of 98.5% was achieved at a gas retention time as low as half an hour which corresponds to extremely high gas flows i.e. 2 m<sup>3</sup> gas per m<sup>3</sup> reactor per hour. The researchers at BioCon also found out that the methanation process was very dynamic and could be very fast re-established after interruption of the H<sub>2</sub> provision. This property is particularly important since cheap renewable H<sub>2</sub> provision could be discontinued in some periods. Intermittent provision of H<sub>2</sub>, with stand-by periods in which no influent gas was provided in the reactor did not deteriorate the process, as the biomethanation efficiency was recovered shortly after reestablishing H<sub>2</sub> provision without any lag-phase. The researchers from BioCon could successfully steer the microbial process by adjusting the nutrient supply to avoid alternative by-products such as acetic acid formation. Samples obtained from three different layers of the packing material, the liquid phase of the reactor and inoculum demonstrated an active biofilm inhabited of hydrogenotrophic archaea which could result in a remarkably high productivity of 10 m<sup>3</sup> CH<sub>4</sub> per m<sup>3</sup> reactor per day, which is 10 times higher than a conventional biorgas reactor.

🔺 Professor Irini Angelidaki



## BioCon

In the Biological Conversions group (BioCon), our goal is to develop and validate novel technologies exploiting microorganisms as tools to transform organic waste and wastewater into useful bioproducts, biofuels, and bioenergy.

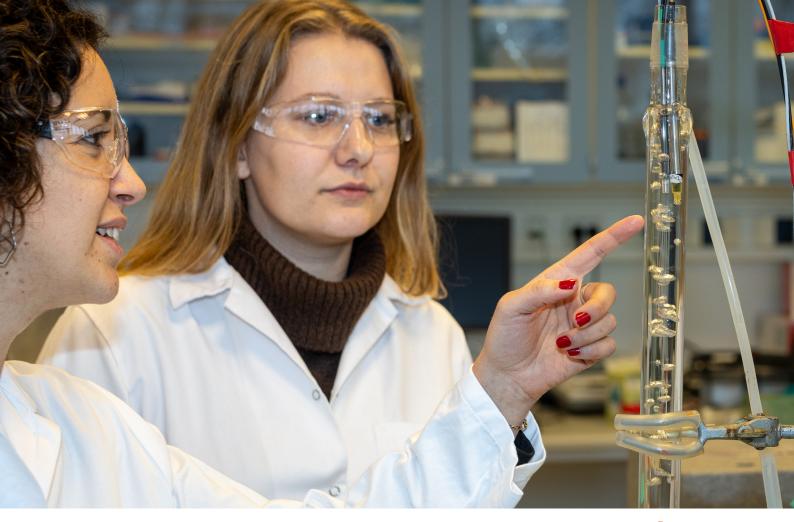
Utilizing our expertise in biochemical engineering, we develop new technologies to upcycle nutrients from residual resources. We start from basic science, uncovering the mechanisms behind microbial processes, and we continue to apply research towards the development of new biotechnological solutions in pilot scale.

Our experience in biological biogas upgrading (biomethanation) can serve as a perfect example of the development of environmentally and techno-economically sustainable solutions at pilot-scale.

Biomethanation activities aim to develop and demonstrate at operational environment advanced, automated, and consolidated concept for CO<sub>2</sub> capture and utilization by exploiting synergies with excess renewable electricity (e.g. from wind turbines, photovoltaic plants) to produce high-grade biomethane equivalent to natural gas (>95 per cent CH<sub>4</sub>) for grid injection. Demonstrating an efficient and high-rate CO<sub>2</sub> capture, utilization and storage technology can markedly combat global warming. In accordance with the European Green Deal to transform EU to climate neutral in 2050, biomethanation can attract growing attention as it can strongly reduce greenhouse gas emissions from industry and energy sectors.

Our ongoing research on biomethanation is focused on increasing biogas production capacity, accelerating start-up period and avoidance of lag phase, revealing proper stand-by mode strategy, unveiling proper dosage, and trickling of nutrients using digested residual resources. In addition, we have increased focus on new reactor configurations, dynamic modelling, and microbial resource management.

The activities are conducted in strong collaboration with wastewater treatment and biogas plants where the biological methanation is evaluated as an alternative methodology to improve economy and sustainability.



PhD students Ariadna Pié Porta and Emilie Overgaard Willer examine the bubble column 👸 Christian Carlsson

## Revisiting the roots of chemical engineering

A new European grant allows Professor John Woodley and colleagues at PROSYS to look at industrially relevant enzyme-based processes with fresh eyes.

Demands for more sustainable processing as well as progress in recombinant DNA technology have led to extraordinary growth in industrial use of bioprocesses. An ERC (European Research Council) Advanced Grant has been awarded to Professor John Woodley at PROSYS for a new project (called FLUIZYME) aiming to look at enzyme-based processes with fresh eyes. Ultimately, the project can lead to improvements in many types of bioprocesses, including those where enzymes and therapeutic proteins are manufactured. While the bioprocess industry already makes significant contributions to global manufacturing, new bioreactions are constantly developed in the laboratory, many of which look very promising for scale-up. Of course, bioprocessing will not replace conventional chemical processes outright, but rather provide a complement, as well as a route to entirely new protein-based medicines and materials.

However, translating these new laboratory discoveries into scalable bioprocesses requires work on how to produce enough product, cheap enough and in a reliable way. Involving around 10 researchers in total, the new ERC Advanced Grant project aims to address these issues using a relatively simple system based on enzyme catalysis.

## Selective oxidation in focus

One of the most difficult reactions for synthetic organic chemists is selective oxidation where strong oxidants are often required. These are reactions that are hard to scale and potentially hazardous, as well as often leading to many by-products, resulting in a loss of yield as well as difficult downstream processing. As it happens, it is also one of the most important reactions in organic synthesis meaning that new substitute reaction methodologies are highly sought after. One possibility is to use molecular oxygen and have enzymes catalyze the reactions. This results in excellent selectivity under mild conditions (neutral pH, atmospheric pressure, and room temperature).

Oxidase, monooxygenase, and dioxygenase enzymes can all be used to carry out oxidations which are useful for industry. Some are relatively simple to use such as oxidases (and others are more complex involving the use of nicotinamide cofactors, which need to be regenerated). However, in all cases oxygen needs to be supplied to the enzyme active site (which can be on the surface of the protein or buried inside where oxygen is transported via channels or tunnels within the protein).

### Bubbles may cause proteins to unfold

Most enzyme reactions are carried out in aqueous solution, which sounds much better than using an organic solvent, till we realize the solubility of oxygen in water is extremely low, around 250 µM (under ambient conditions in equilibrium with air). This means that oxygen needs to be continually supplied via bubbling, and this is where biochemical engineering science begins. What happens to enzymes at the surface of an oxygen bubble (as they rise through a column)? How important is the size of the bubble? What happens to the bubble when it bursts at the surface?

It is well known that proteins can unfold at hydrophobic interfaces such as gas bubbles, but how fast is that unfolding and what happens afterwards to the protein? These questions are still unanswered, and in the FLUIZYME project a team of researchers are now investigating the answers using scaledown apparatus (miniature bubble columns and chromatography) to help build models of the phenomena, later as the basis for integrating with kinetics and predicting scale-up.

### Gradients in large tanks

The implications go far beyond bubbling. It has been known since the 1970s that proteins in solution can unfold when the solution is stirred. Given the size of proteins it is not due to mixing. However, air drawn down from the surface is believed to have an impact in denaturing the proteins. This has implications for many types of bioprocesses, including those where proteins are manufactured (either as enzymes, such as in Novozymes or say biopharmaceutical products, such as in Novo Nordisk).

The new project also aims to study scale-up effects related to concentration gradients in large tanks. Gradients have effects on kinetics and stability of enzymes. Such effects can also be seen in reactions requiring pH control or addition of otherwise inhibitory substrates (at the high concentrations required). In the case of enzymes, the rate law of the reactions means that the observed rate is often quite sensitive to the substrate concentration.

Likewise, enzyme reactions (released from the constraints of working in a cell) can catalyze reactions orders-of-magnitude faster than fermentations. Even at a volumetric rate of 20 g/L.h, the gradients seen in a tank will be considerable and have effects not only on kinetics but also longterm stability. Again scale-down apparatus is being used in the project to test such effects and will ultimately be modelled and the predictions (also using SFD) will be validated in the Pilot Plant at DTU Chemical Engineering.

Postdoc Elif Erdem and Professor John Woodley

## **Biochemical engineering science**

By the 1950s and 1960s, chemical engineers had succeeded in implementing many new industrial processes, taking basic chemical reactions from laboratory to large-scale process plant. Along the way not only was process control required so that products could be produced in specification, but phenomena in the various reactors and unit operations were studied in detail. This included residence time distribution in reactors (pioneered by Danckwerts at Cambridge, UK), and other phenomena such as fluidization (pioneered by Davidson, also at Cambridge) to name a few. Later, work on bubble columns and other operations were considered. The chemical engineers that promoted this aspect of our discipline, and the associated mathematics, termed it 'chemical engineering science', primarily to distinguish it from process design and optimization.

FLUIZYME, the new ERC Advanced Grant project on bioprocesses, aims to go back to the roots of chemical engineering, now with fresh eyes on enzyme-based processes. One of the most fascinating developments in enzyme catalysis (biocatalysis) is the ability to swap amino acids in the enzyme, altering the properties. Indeed, protein engineering as it is termed earned a Nobel Prize for Frances Arnold from Caltech in 2018.

If the scale-down techniques developed in FLUIZYME could be made even smaller (microfluidic) such that thousands of enzyme variants could be screened, the approach developed here could also be used not only to predict large-scale performance of enzyme-catalyzed reactions, but also allow screening to establish the best enzyme to be used at a larger scale.

## PROSYS

Our main purpose is to perform research and teaching that will contribute to developing technologies for future more sustainable chemical and bio-based production processes.

Furthermore, our activities include digitalization of production processes as well as societal challenges by addressing several Sustainable Development Goals (SDGs), most importantly sustainable production and consumption (SDG12), climate action (SDG13) and affordable and clean energy (SDG7).

Our research work, often in collaboration with industrial partners, involves two main components: **Process systems engineering (PSE)** 

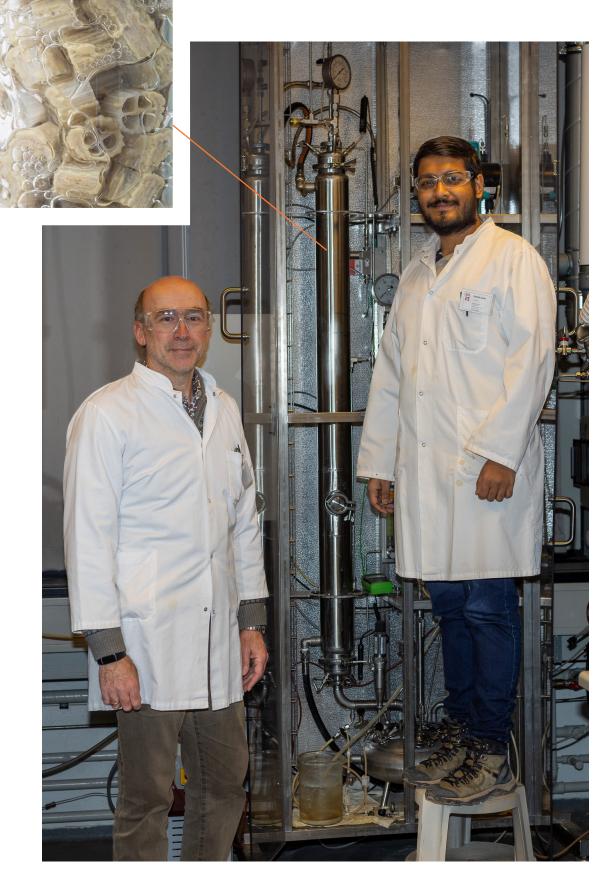
We develop computer-aided tools for a broad range of processes including food and pharma production, manufacturing of chemicals and wastewater treatment/resource recovery. We work with mathematical modelling and simulation, optimization, process synthesis and design, etc. In recent years, Life Cycle Analysis (LCA) has developed into an important tool complementing traditional techno-economic analysis of process alternatives. **Bio-based processes (biocatalysis, fermentation and downstream processing)** We perform experimental and theoretical work that spans from microscale over lab and pilot-scale to full-scale activities, also including digitalization of the systems studied.

Within fermentation, we work with pure and mixed cultures, and we have also developed activities involving scaling up/scaling down, computational fluid dynamics, and develop-ment/test of novel online sensors.

In biocatalysis, multi-step biocatalysis and in-situ product removal (ISPR) are investigated, as well as oxygen supply methods for bio-oxidations. Enzymes investigated include alcohol oxidases, carbohydrate oxidases, cytochrome P450s, Baeyer-Villiger monooxygenases, dehydrogenases, peroxidases, laccases, and transaminases.

Within downstream processing, we cover a broad range of unit operations (e.g. distillation, crystallization, extraction, chromatography), for example investigating methods to obtain improved control of such processes, and have detailed expertise on different applications of membrane processes, particularly classical liquid operations—from microfiltration to reverse osmosis—and use of membranes for enzyme immobilization.

Collaboration is key to our existence, and therefore PROSYS has many international academic partners, and participates in a broad range of industry collaborations. At the Department, we have frequent collaborations with PILOT.



Ph.D. student Sambit Dutta and supervisor Assoc. Professor Ioannis V. Skiadas next to a pilot installation of a TBR for syngas biomethanation. Picture on the left showing an inside view of the bioreactor.

## Scaling-up of syngas bioconversion to green methane

Through modelling of variable mass transfer and reactor hydraulics for optimal upscaling, efficient fermentation of syngas is being accomplished. The end-product is biomethane with a 98 % CH<sub>4</sub> content which corresponds to natural gas grid quality.

Biomethane has the potential to replace fossil derived CH<sub>4</sub> (methane, also known as natural gas) in the global gas grid. Researchers at DTU Chemical and Biochemical Engineering have succeeded in producing biomethane through gas fermentation. The product has more than 98% CH<sub>4</sub> content, which corresponds to grid quality. Feedstock for the process is syngas, which is a mixture of H<sub>2</sub>, CO<sub>2</sub>, and CO. The syngas can be produced from either biomass gasification or pyrolysis.

In the project, a trickle bed reactor (TBR), which is a type of packed bed reactor, was used. PhD Student Sambit Dutta, Pilot Plant, DTU Chemical and Biochemical Engineering, is developing the modelling tool for optimal scaling-up of the TBR for syngas biomethanation.

"This reactor type is advantageous due to high surface area-to-volume ratio, which facilitates efficient mass transfer of gaseous substrates from gas phase to liquid phase. In the project, the TBR proved able to fully convert  $H_2$  and CO in the syngas. When additional  $H_2$  is added, more than 98% CH<sub>4</sub> in the product can be achieved," says Associate Professor Ioannis Skiadas, Pilot Plant, heading the project.

## Mild conditions benefit economy

Microbial kinetics and biothermodynamics have been extensively studied in collaboration between Pilot Plant and AT-CERE, also at DTU Chemical and Biochemical Engineering. Both laboratory and pilot scale TBRs were inoculated with mixed microbial consortia which were immobilized by forming biofilm on the packing material and were fed syngas and nutrients for performing syngas biomethanation at optimum temperature and pH.

"Despite the higher complexity of microbial consortia compared to pure cultures, the mixed culture approach presented a series of inherent merits such as non-sterile operation, higher adaptation capacity, higher tolerance to the impurities of the raw syngas, and resilience after a disturbance in operating conditions," says Associate Professor Hariklia Gavala, AT-CERE.

These advantages are substantial when it comes to maintaining the productivity of a continuous process, explains Hariklia Gavala:

"Moreover, the results were obtained under mild conditions, meaning ambient pressure and temperature, which greatly benefits the economic feasibility of the process."

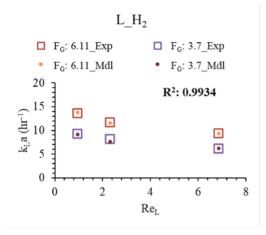
### Next step: optimization tool

Notably, the same reactor configuration is suitable for the fermentation of not only syngas but also CO<sub>2</sub> if combined with H<sub>2</sub>. However, due to its complexity (different reactor and packing material geometries, mass transfer limitations, complex liquid, and gas flow patterns, three-dimensional microbial growth in biofilm, biofilm mechanical structure and stability) the efficiency of the process is difficult to predict at different sizes and TBR configurations.

The process has been brought to pilot scale and further work needs to be done. "There are still certain challenges preventing us from scaling up the process to demonstration or production scale," notes loannis Skiadas.

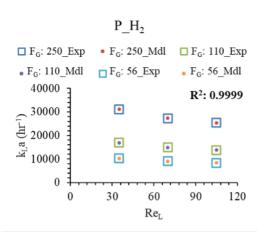
"Therefore, ongoing work in Pilot Plant focuses on developing a simulation tool able to predict the efficiency of the TBR as a function of size, reactor aspect ratio, packing material, gas and liquid flow rates. Presently, a model is being developed by incorporating microbial kinetics and volumetric mass transfer rates to simulate the overall fermentation process for lab and pilot scale TBR. The goal is to develop a universal model for both TBR scales which will allow optimal design and scale-up of TBR methanation units."

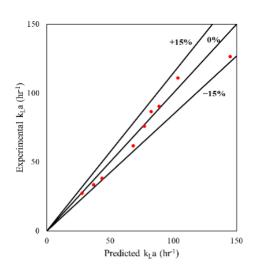
Associate Professor Ioannis Skiadas



The figure above presents a model to predict the mass transfer coefficient ( $k_L$ a) of  $H_2$  in water in the lab (L) and pilot (P) scale TBR at different liquid flowrates represented by liquid Reynolds number (Re<sub>L</sub>) and different gas flowrates (FG, ml/min).

Based on the accuracy of the dimensionless equation to predict the  $k_{L}a$  at both lab and pilot scale TBRs, the model can allow calculations for the scaling up of the process. Then, optimization of operating parameters such as gas and liquid flowrates and reactor configuration must be conducted before further scaling up. Although model development is still ongoing, preliminary simulation results are promising since the model was able to predict the  $k_{L}a$  of a pilot scale TBR very accurately, based on experiments performed on lab scale TBR as shown in the figure to the right. Based on simulation predictions, economic feasibility and life cycle assessment of the overall process will be also carried out which will provide valuable information to the industries interested in setting up commercial scale syngas biomethanation units.





## PILOT

The DTU Chemical Engineering Pilot Plant offers and further develops our unique equipment infrastructure and our strong theoretical and practical unit operation competences within existing and state of the art technologies and processes of the chemical, pharma, biotech, food and energy industries.

Our aim is to provide world-class education for the students, and to be the most attractive research partner for our employees and for industry, educational institutions and society. The recent major expansion of the Department's pilot halls, laboratories and process and analytical equipment will ensure that our educational and research facilities and its activities will be even more attractive, modern and efficient.

With four new large pilot halls in addition to the existing five halls, and a huge investment in new process and analytical equipment, we are able to operate, simulate, and develop many types of unit operations and process lines in pilot scale, representing the life science industry as well as traditional chemical, biochemical and food industries.

A major investment in the digitalization of a significant part of our pilot units has been implemented during 2022-23. The project includes implementation of a Siemens Scada system for educational and research data collection and manipulation, and a virtual reality environment for e-learning to facilitate the remote study of some of the most used unit operations.

A new pilot scale fermentation-based manufacturing line for pharmaceuticals, food and biochemicals, including fermenters from lab scale to 250 litres, and a broad selection of relevant downstream separation and purification equipment, has been approved for hand-ling of Genetically Modified Organisms class 1 in large scale. Furthermore, we have the amplest lab facilities also approved for GMO projects.

We are focusing on attracting new external collaborators to increase our research and innovation activities based on processes, technologies and equipment. This will continue to enhance a dynamic interface and activity between our capabilities and our existing and new external collaborators.

## KT Consortium advances software tools for productprocess modeling and thermodynamics

As a member of KT Consortium, companies can get access to software tools that can advance industrial processes and optimize performance

KT Consortium, a cross-section center affiliated with DTU Chemical Engineering, collaborates closely with industry partners to promote cutting-edge software tools in the field of product-process modeling, simulation, and thermodynamics. ICAS is the most wellknown and oldest tool, while the newest addition, eThermo, is set to launch in the spring of 2024. eThermo has a specialized focus on electrolyte systems thermodynamics. Besides software tools, another focus for KT Consortium is participating in research machine learning (ML) for property prediction.

## **ICAS - A legacy of evolution**

ICAS, short for Integrated Computer Aided System, has evolved significantly since its beginning at DTU Chemical Engineering several years ago with the first paper presenting ICAS dating back to 1997. Initially built to consolidate existing tools at the department, ICAS has transformed over the years into a comprehensive standalone tool for simulating continuous and batch processes in both steady or dynamic states, with or without controllers.

The early versions of ICAS included five toolboxes addressing different tasks of pro-

cess simulation. Over the years, additional toolboxes have been integrated, while the existing ones have been further developed and can now be used also as standalone tools via ICAS task manager. One such example is ProPred, initially part of the thermodynamic toolbox, which is used for the property prediction of pure compounds. ICAS task manager includes additional modules, such as ProCAMD, dedicated to computer-aided molecular design, SolventPro, dedicated to solvent design, ModFrame used for model development, Thermodynamic Model Selection, Process Design Studio, and ProCAFD used for process synthesis.

The latest ICAS release, ICAS v.25.0, launched in June 2023 comes with several bug fixes and new flammability property models implemented in ProPred. The plan for ICAS development in forthcoming years focuses on the implementation of novel property models and the enhancement of existing modules to ensure increased robustness.

## eThermo - A new tool for electrolyte property simulation

In September 2023, DTU granted a Discovery Grant to Software Manager Andre Vinhal,

DTU Chemical Engineering, to develop a prototype software tool for simulating the thermodynamic properties of electrolytes using an advanced equation of state (EoS). This software consists of a thermodynamic package featuring the EoS, a database of experimental data, and model parameters for key electrolyte components, all accessible through a user-friendly interface. Developed under the ERC Advanced Grant ElectroThermo, the model and its parameters exhibited exceptional performance, accurately representing the thermodynamic properties of electrolyte solutions across aqueous, non-aqueous solvents, and mixed solvents.

The prototype of the tool allows the user to calculate the mean ionic activity coefficient and densities for various solvents and salts. The users can compare these results with experimental data stored in the database and generate comprehensive reports. This marks the initial phase in the design and programming of a complete software solution for simulating diverse electrolyte systems, with upcoming features set to include phase behavior evaluation and features to allow interaction with process simulators.

## Machine Learning for property prediction

Building on the long-standing history of developing property models for pure component properties at the department, KT Consortium has embraced recent years' developments in the field of AI/ML to strengthen its position as a leading research institute in the field. KT Consortium alongside the department has funded the PhD project "Machine Learning and Deep Learning Applications for New and Improved Property Predictions".

These newly developed approaches allow the user to overcome many of the drawbacks of the existing methods such as low accuracy and limited domain of applicabil-



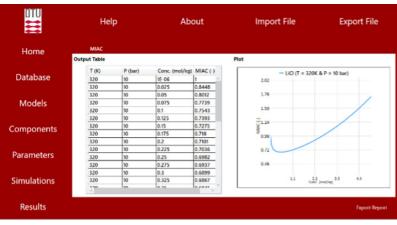


Figure 1. e-Thermo screenshots

ity. The model developed by Postdoc Adem R.N. Aouichaoui is a state-of-theart ML model that incorporates fundamental in-house chemistry knowledge (in the form of functional groups from group contribution methods). This is the only ML model that covers over 30 physiochemical and safety properties, and 19 temperature-dependent properties and has been ranked as one of the best deep learning models for these types of applications. Initial investigations into prerequisites for implementing such models as online solutions reveal promising potential.

These examples are just some of the many initiatives at KT Consortium in its efforts to develop tools and conduct research relevant to its company members.

## **KT Consortium**

At KT Consortium we bring together advances and developments made in the area of Process Systems Engineering, Bio-Process Engineering, Applied Thermodynamics and Property Prediction within the Department of Chemical and Biochemical Engineering at DTU and to continuously improve and innovate for a better and more sustainable future.

The KT Consortium is an industry-academia collaboration providing service to company members by fostering a cross-sectorial understanding of (Bio-)Process Systems Engineering and Thermodynamics. The consortium was founded in 2017 based on a long-standing history of collaboration with industry from previous centres and consortia at the Chemical and Biochemical Engineering Department.

We work on developing generic methods and tools using computer-aided systems approach to solve and analyse problems related to product-process modelling, simulation, synthesis, design, analysis, control, and operation for companies within the areas of chemical, pharmaceutical, agrochemical, food, and biochemical industry. KT Consortium is a cross centre activity involving faculty and students from AT-CERE, PROSYS and CHEC research centres. We have close collaborations on a number of projects, work together in funding applications and for supporting our member companies on a wide area of assignments.

As an industrial member of the KT Consortium, one will be provided with state-ofthe-art CAPE and PSE methods and tools, the technologies for future chemical and biological processes along with a series of other benefits such as:

- 1. Participation in the Annual Meeting
- 2. Web access (via dedicated members site) to:
  - Manuscripts in advance of publication
  - PhD theses (including online defences)
  - ICAS software
  - ICAS training courses
  - Chemical Databases (Electrolyte, IL, organic compounds, etc.)
  - Annual Meetings materials (videos, presentations, workshops)
  - Online seminars (live and recorded) from KT Consortium affiliated staff and faculty as well as invited guests from around the world supported by CERE and PROSYS research centres.
- 3. Access to collaboration and research from:
  - Student projects
  - Visiting PhD students
  - Joint Research Projects
- 4. Access to know-how and influence on the research programme.

If you are interested to join KT Consortium or know more about, please contact Professor. Georgios M. Kontogeorgis.

## Highlights **2023**

## 17 JANUARY GREEN TRANSITION CONFERENCE

The conference for Innomission 1 and Innomission 2 MissionGreenFuels took place at DTU. CHEC, via Prof. Anker Degn Jensen and Assoc. Prof. Martin Høj, participate in MissionGreen-Fuels with the sub-project Methanol-to-jet fuel process. The aim is to make jet fuel from methanol along with partners Ørsted, Topsoe, SkyNRG, Neste, Aalborg University, Copenhagen Airport, NISA, SAS, and Aarhus University.

## 25 JANUARY

## SEMINAR ON QUANTUM COMPUTING

At the first departmental seminar of the year, Christopher Savoie, CEO of Zapata Computing, spoke about the recent progress in quantum computing research. He is a published scholar in medicine, biochemistry, and computer science and the original inventor of AAOSA, the A.I.-based natural language interface technology used to develop Apple's Siri. He visited the department because Zapata Computing is funding a PhD student at DTU Chemical Engineering due to a common project in quantum computing.



### 9 FEBRUARY

## VISIT FROM MAERSK DECARBONISATION

Our department hosted 50 visitors from Maersk Decarbonisation of A.P. Møller Mærsk. Besides a tour of the department, members of our faculty gave presentations on de-carbonisation, sustainable production of fuel for the maritime sector as well as the use of alternative fuel in the maritime sector.

## 2 MARCH DTU OPEN HOUSE

2,000 visitors made their way past the DTU Open House, which, among other things, offered an education fair, tours and lectures with fully qualified engineers. In the sports hall, students and teachers stand ready at the stands, lined up with effects designed to attract curious young people to DTU's various educations, courses and offers.

## 28 MARCH

## VISIT FROM DTU'S CHAIRMAN OF THE BOARD

DTU's Chairman of the Board, Karin Markides, Prof., and President of American University of Armenia, visited DTU Chemical Engineering on one of the last wintery days of March. She was shown around the department, including Pilot Plant, and met with center leaders to hear about the department's key research areas.



## 21 APRIL VIP VISITS TO OUR PILOT PLANT

Senior Vice President for Innovation and Entrepreneurship at DTU, Marianne Thellersen, visited DTU Chemical Engineering to hear about our digitalization strategy, and see it live at our Pilot Plant. Perspectives for the digitalization at DTU were also discussed. Throughout 2023, private companies also visited us to learn about the digitalization of our Pilot Plant, including Alfa Laval and Novozymes.

## 25 APRIL Coast Annual Day

The Hempel Foundation Coatings Science and Technology Centre, CoaST, held their 6th Annual Day highlighting the latest in coating research. 87 participants heard a series of oral presentations by PhD students and guest speakers included Vice President for R&D, Nigel Shewring from Hempel A/S.

## Highlights **2023**

## 25 APRIL

## THE HEMPEL-DTU AWARD

Congratulations to HTX Roskilde for winning the Hempel Foundation & DTU Forskerskolepris for their special effort for the STEM subjects. The jury highlighted the school's particular focus on STEM didactics which is important to make more students interested in the STEM subjects.

## 10-12 MAY

## QUANTUM COMPUTING APPLICATIONS WORKSHOP

The workshop brought together scientists and engineers at all career stages in academia, industry, and startups to display advances in the emerging and rapidly growing field of quantum computing. Top researchers and experts on QC such as Prof. Prineha Narang, Jhonathan Romero Fontalvo of Zapata Computing, Inc., and Prof. Fred Chong shared their knowledge and new collaborations were initiated. Assoc. Prof. Soheil Mansouri from DTU Chemical and Biochemical Engineering chaired the workshop.

## 26 MAY

## **40-YEAR WORK ANNIVERSARY**

Almost 200 well-wishers turned up to congratulate our Head of Department, Prof. Kim Dam-Johansen on his 40 years' work anniversary at DTU Chemical Engineering, which was on 1 February 2023. President of DTU Anders Bjarklev gave a speech honoring Kim's many achievements for both our department and DTU.



## ) MAY

## DTU MICROBES CONFERENCE

Asst. Prof. Julian Kager from DTU Chemical Engineering gave a presentation about fermentation platforms and capacity at DTU at the DTU Microbes Conference held at DTU Biosustain. The conference brought together DTU researchers, alumni, industry professionals, and other experts to explore the latest insights, technologies, innovations, and solutions in microbes-related research.

## 2 JUNE SECOND FBM SYMPOSIUM

The Oticon Hall at DTU was buzzing when new insights on biomanufacturing were presented and discussed at the second symposium of the FBM-Initiative: "Innovation for Biomanufacturing – New Processing technologies towards sustainable and Automated Industry." More than 200 participants registered for the event.

## 7-9 JUNE CERE DISCUSSION MEETING

109 members of the CERE industry consortium met at Marienlyst Strandhotel in Helsingør to discuss the wave of transition in the energy resources sector with focus on thermodynamics and  $CO_2$  capture.

## 0-12 JUNE

## **KT CONSORTIUM ANNUAL MEETING**

Fifty members, both internal and external, attended this year's KT Consortium Annual Meeting 2023. They discussed process and bio-process systems engineering with researchers from DTU Chemical Engineering.

## 17 JUNE UNF VISIT

Ungdommens Naturvidenskabelige Forskning, UNF, visited our department as part of their Chemistry Camp 2023. 86 high school students and volunteers from DTU attended lectures, classes, study assignments and trips to see what an education in chemistry entails. At our department, the students experienced chemistry on a large scale in our Pilot Plant and toured our centers, CoaST, CHEC and AT CERE.

#### 30 JUNE ERC ADVANCED GRANT FOR PROF. IRINI ANGELIDAKI

Prof. Irini Angelidaki from DTU Chemical Engineering received the prestigious Advanced Grant from ERC, the European Research Council. The grant of EUR 2.5 m will for the next five years fund research in a completely new way of performing fermentations with designer microbial consortia. This will have an impact on future technologies for using residual biomasses to produce bioproducts, biochemicals and bioenergy.



#### 4-28 JULY SUMMER UNIVERSITY

Another summer, another summer university at KT's pilot plant. This year 54 students, primarily from the USA, participated. The course within large scale chemical unit operations is specially designed for international and non DTU students.

# 7 JULY VISIT FROM SOUTH KOREA

A South Korean delegation from 4 Universities/institutions visited DTU Chemical Engineering. At a workshop they presented their activities within Environmental Biotechnology and  $CO_2$  capturing technologies.

#### 18 JULY PhD WINS THE 2022 MOLECULAR PHYS-ICS EARLY CAREER RESEARCHERS PRIZE

From all the nominations for the 2022 Molecular Physics Early Career Researcher Prizes, the panel of Editors chose PhD student Gabriel M. Silva's paper "On the derivations of the Debye-Hückel Equations" out of two prizes awarded. The paper was deemed to exhibit an excellent standard and of particular interest to the readers. Co-authors are Assoc. Prof. Xiaodong Liang and Prof. Georgios M. Kontogeorgis, and the article was published in Molecular Physics 120 (9-10).

### 21 AUGUST **KT RESEARCH DAY**

DTU Chemical Engineering held its annual KT Research Day. Head of DTU Compute, Jan Larsen, gave a highly topical talk about "How CHATGPT is expected to influence universities" educations and research" and PhD students Adem R.N. Aouichaoui and Marcel Butschle won the poster and pitch competition.



### 21-25 AUGUST PhD SUMMER SCHOOL

Gürkan Sin held a weeklong Summer School on Uncertainty and Sensitivity Analysis of Model Output in Engineering Applications for 35 PhD students in August.

# Highlights 2023

#### 18-22 SEPTEMBER BIOPRO WORLD TALENT CAMPUS ANNIVERSARY

The 10th edition of BIOPRO World Talent Campus was organized in Sorø for 25 international PhD students. The participants come from leading universities around the world. The World Talent Campus is sponsored by the Novo Nordisk Foundation and the BIOPRO partners.

#### 30 SEPTEMBER

# DPC ANNUAL POLYMER DAY

The DPC Annual Polymer Day was attended by 89 participants. Prof. Jukka Seppälä from Aalto University gave this year's international research presentation on the topic of biobased polyesters and polyamides for bio-composites. Other research presentations and a poster session followed.

#### 5 OCTOBER CHEC ANNUAL DAY

30 external and 50 internal guests attended the CHEC Annual Day which featured presentations from industrial collaborators KVASIR Technologies, Mash Makes, Lundbeck, Ørsted and Alfa Laval as well as research presentations on catalysis and high temperature processes.

# 13 OCTOBER

# PROSYS RESEARCH SEMINAR

187 participants, hereof 87 industrial participants, attended the 7th PROSYS Research Seminar, an informal networking event to share the latest developments and highlights from PROSYS research activities. Guest speakers this year were from GEA, FUJIFILM Diosynth Biotechnologies and the University of Sydney.

#### 30-31 OCTOBER AIM-Bio SYMPOSIUM

DTU Chemical and Biochemical Engineering hosted the AIM-Bio symposium 2023. For two days, the 70 participants heard speakers, poster presentations and experienced The Biotech City in Kalundborg. The AIM-Bio project unites DTU and North Carolina State University's academic powerhouses for innovation in biomanufacturing.



# 15 NOVEMBER BEST OF THE BEST POSTER AWARD

Amongst 75 works presented at the Danish Offshore Technology Conference 2023, Postdoc Magdalena Skowyra and PhD student Maria Echarri Giacchi's poster was awarded 'The best of the best' poster. Their work touches upon a more sustainable way of plug & abandonment of oil wells using a novel polymer material.

### 16 NOVEMBER 25-YEAR WORK ANNIVERSARIES

Our Head of workshop, Søren Vestergaard Madsen, celebrated 25 years working at DTU Chemical Engineering. Søren has played a pivotal role in shaping the evolution of the workshop into its current state. This year Chief Consultant, Lisbeth Degn from the department secretariat, and Senior Researcher, Anne Juul Damø from the CHEC center, also celebrated their 25-year anniversary at DTU Chemical Engineering.



#### 17 NOVEMBER VISIT FROM IAPAN

A delegation of eight visitors from five large Japanese companies (Osaka Gas, Hitachi, Kawasaki Heavy Industries, Takuma, and EX Research Institute), visited DTU Chemical Engineering. At a workshop, the Japanese delegation and Biocon researchers presented their activities and interests within CO<sub>2</sub> capture novel technologies.

#### 17 NOVEMBER

#### YOUNG RESEARCHERS AWARD

DTU celebrated this year's PhD graduates at DTU at a party that combined the awarding of diplomas with awards. Isaac Appelquist Løge, won a Young Researchers Awards for his thesis: 'The Kinetics of Scale Formation.'

### 27 NOVEMBER

# INAUGURATION OF CO2 PILOT PLANT

A big day for Assoc. Prof. Philip Loldrup Fosbøl, when he and his teams'  $CO_2$  capture pilot plant was inaugurated by HRH Crown Prince Frederik at Aalborg Portland A/S. Other notabilities at the event were European Commissioner Kadri Simson and Lars Aagaard, Danish Minister for Climate, Energy and Utilities. With this plant, an innovative technology within  $CO_2$  capture is tested that can potentially eliminate a significant part of the energy consumption in  $CO_2$  capture and ensure better utilization of the collected  $CO_2$ .



💿 European Union, 2023

# 8 DECEMBER KT CHRISTMAS SEMINAR

Prof. Anja Boisen from DTU Health Tech gave a presentation on her experiences with spinout companies at the KT Christmas Seminar. The centers at KT also presented a selection of their research results during another successful year at DTU Chemical Engineering.



# 11 DECEMBER NEW MILLING MACHINE

The workshop at DTU Chemical Engineering assists the researchers at our department in developing new instruments and designing processes. At the end of the year, the workshop received its new state of the art milling machine. It will be able to mill steel into every size and shape and is a major upgrade of the workshop's machine park.



# Cooperating companies

#### 2 21st

21<sup>st</sup>.Bio

# 3

3V TECH EQUIPMENT & PROCESS SYSTEMS SPA A AGC Biologics Air Products Alfa Laval A/S Algiecel ApS ALK Abello A/S Amager ressource Center Aquaporin A/S ARKEMA FRANCE Arla Foods Ingredients Group P/S AVEVA Avista Green AWAPATENT

# В

Axens SA

Baker Hughes BASF Bayer Beyond Leather Materials BioLean Biomar Bioscavenge ApS Biosyntia Bjørn Thorsen A/S BP

# С

Calsep Carbfix Centro Tecnológico Componentes Chevron Chr Hansen A/S Chreto A/S Chromologics ApS Ckj Steel A/S C-LEcta Coloplast A/S Copenhagen Atomics Covestro Deutschland AG CP Kelco

# D

Dalum Danfoss Dansk Gasteknisk center A/S Dan-Unity A/S DHI DSM-Firmenich

ECCO Elkem EnCoat Enduro Engineering Consulting Corporation ENI EnviDan A/S Equinor ESSS North America

# F

Fluor Corporation Fuji Pharma Fujifilm Diosynth biotechnologies

# G

G2B Biosolutions ApS GEA Process Engineering A/S GN Hearing Aid GR3N SAGL Greenlab Skive Carlsberg Research Laboratory Grundfos

# н

Hafnium Labs Topsoe A/S Haper & Vedel Harriot Wiat Hashøj HCS Hempel A/S Henkel AG HENNES & MAURITZ (H&M) AB Hillerød Forsyning Holm Christensen Biosystemer ApS Hundested Havn HUTCHINSON

# T

IFP Energies nouvelles IFPEN INNARGI A/S Innosyn Insatech A/S

# J

Johnson & Johnson Innovative Medicine

# K

Kaffe Bueno ApS Kalundborg forsyning A/S Karup Kartoffelmelsfabrik KBC KMT Cables

# L

Landbrug & Fødevarer FmbA LEGO Lemvig Biogas Leo Pharma Linde LiqTech International Lucent Petroleum Lundbeck Pharma A/S Lundsby Biogas A/S

# Μ

Madsen Bioenergi I/S Media Medic Metricorr Microsoft Mitsubishi Chemical Corporation Momentive Mölnlycke

# N

NEO GROUP Neste Corporation New Energy Coalition Nilpeter Nopa Nordic Sugar A/S Nouryon Specialty Chemicals B.V. Nova Pangeae Novo Nordisk A/S Novozymes A/S

# 0

Octarine Bio A/S OMV Petrom

# Р

ParticleTech ApS Pharmacosmos Polyloop Pond Process-design A/S PROCESSI INNOVATIVI SRL Processium

# Q

Q-Interline

# R

Rambøll A/S Resino Ringsted Forsyning River Stone Biotech ApS Rockwool A/S Roxtec

# S

Saltkraft A/S SaltPower Schlumberger Scienciox Scott Sports Shell Sinopec Skanderborg Forsyning Skovgaard invest SMK (Statens Museum for Kunst) SpectroInlets ApS SYNESIS Syngenta

# Т

Tetrapharm TotalEnergies Tårnby Forsyning

# U

Unibio Group Unilever Union Engineering US Navy

# ١

Vandcenter Syd Viegand & Maagøe Viking Malt

# W

Waste Plastic upcycling Wetsus Wintershall

#### X Xellia Pharmaceuticals

Z Zapata Al

Ø Ørsted A/S

Aa Aalborg Portland

# **Expanding KT Students**

The student organization at DTU Chemical Engineering, KT Students, aims to create an engaging study environment for students through social and professional activities. In 2023, the goal for KT Students was to integrate more students, and strengthen know-ledge sharing in chemical engineering organizations across the Nordics.

In the spring of 2023, the focus of KT Students was to arrange company presentations at DTU, giving chemical engineering students an insight into diverse company profiles.

"DTU has the advantage of having many available resources and connections to the chemical and biochemical industry. Fostering a relationship between the professional world and academia, is beneficial both for students wanting a closer look at what their future could look like, as well as for companies to be inspired by future engineers." says Melissa Jensen, Chairman of KT Students.

In October 2023, KT Students participated in the Nordisk Kemiteknik Konference (NKK), a student conference in Lund. Here, various chemical engineering organizations from the Nordic countries came together to collaborate, network, and exchange ideas. The event was successful and included several lectures from chemical engineering professors at Lund University as well as visits to the Lund University pilot plant and food technology laboratories.

Currently KT Students are working towards inspiring more Bachelor of Engineering Students to join the organization, as the majority today are master students.

DTU is a highly esteemed university worldwide. This is something KT Students take pride in. Just as DTU Chemical Engineering strives to be among the best, KT Students as a student organization, also aim at being among the best.

### 🐣 Melissa Fernanda Rugholm jensen



KT Students members and board members attending NKK. From left to right (top then bottom row). Kasper Jørgensen, Laura Karlsmose, Mikkel Stub Neubert, Emilie Tage Andresen, Aske Hansen, Alexander Bonde Skov, Emil Blicher Hansen, Nikolaj Falkenberg, Magnus Banke Johansen, Janie Dittmann Weimar Andersen, Mathilde Munch Jensen, and Melissa Fernanda Rugholm Jensen. Or Ragne Sandell

# Organization

					COMMIT	
LEADER GROU		DF DEPARTMENT	ADVISORY BC	JARU		TEES / BOARDS
		Dam-Johansen	Lars Bang			d (elected/appointed)
Head of Secretar			Per Falholt			rch & Innovation
Head of Study Comn	nittee		Susanne Grø			ation (appointed)
			Michael Hallgre	een		rironment (elected)
			Katarina Lindst			mmittee (elected)
			Carsten Risberg	Lund	Cyber S	ecurity Committe
			Hanne Everla	nd	(	appointed)
STUDY COMMIT	TEE		SECRETARIAT & BI	UILDINGS	W	ORKSHOP
Anker D. Jenser	1		Mette Bjørnlu	ind	Søren Ve	stergaard Madsen
MSc Petroleum Enginee MSc Chemical & Bioche MSc Chemical & Bioche Ind. MSc Biomanufactu	mical Engineering mical Engineering (SD	C)				
		FAC	ПТΛ			
AT CERE	PROSYS	CHEC	CoaST	DPC		BioCon
Georgios Kontogeorgis	Krist V. Gernaey	Kim Dam-Johansen/ Anker Degn Jensen	Kim Dam-Johansen	Anne Ladega	ard Skov	Irini Angelidaki
PILOT Steen Larsen						
	and to Kantana i					
KT CONSORTIUM Ge	orgios kontogeorgis	>				

# The Faculty **2023**

### SCIENTIFIC





Anders E. Daugaard Associate Professor

Anne Ladegaard Skov Professor

Anker D. Jensen Professor









Hao Wu Associate Professor

Hariklia N. Gavala Associate Professor



Helena Junicke Associate Professor



Ioannis V. Skiadas Associate Professor



Irini Angelidaki Professor



Jakob K. Huusom Associate Professor



Jakob M. Christensen Associate Professor







John Woodley Professor



Julian Kager Assistant Professor Professor Head of Department



Krist V. Gernaey Professor

Seyed S. Mansouri Associate Professor



Søren Kiil Professor



Martin Høj Associate Professor



Nicolas von Solms Professor







Philip L. Fosbøl Associate Professor

# **TECHNICAL AND ADMINISTRATIVE**



Mette Bjørnlund Head of Secretariat



# **EMERITUS**



Emeritus

Gunnar E. Jonsson Associate Professor Kaj Thomsen Emeritus



Ole Hassager Professor Emeritus



Sten B. Jørgensen Professor Emeritus



Stig Wedel Associate Professor





Xiaodong I Associate



iang Professor		





# Advisory Board



LARS BANG EXECUTIVE VICE PRESIDENT H. LUNDBECK A/S

"Every day serving more than 7m patients with brain diseases around the globe from European factories requires competitive technological solutions. Our partnership with DTU Chemical Engineering is a cornerstone in developing solutions that really make a difference and is attracting talented new employees."



HANNE EVERLAND VICE PRESIDENT EMENDO R&D APS

"As Senior consultant at Emendo Consulting Group, I service the Danish medical device industry broadly. Here I see how innovation is promoted by collaborations with DTU Chemical Engineering and I meet remarkably knowledgeable students and graduates from the department. Plastic are the main components of most medical devices and with the increased focus on the environment impact of plastic the Danish Polymer Center is an important partner for the industry in the development of new and more sustainable polymers."



PER FALHOLT CHIEF SCIENTIFIC OFFICER 21<sup>ST</sup>.BIO

"I am a biotech entrepreneur with a long experience from launching industrial biotech products to many different industries, food, feed and technical. With my experience from Industry combined with my DTU insight from being Chairman of the board at DTU I can bring relevant societal needs and challenges into our research and education environment at Chemical Engineering and will use this to help educate the relevant candidates for the future."



SUSANNE GRØN VICE PRESIDENT FOR R&D PROCESS SCIENCE & DEVELOPMENT CHR. HANSEN

"Climate change, food waste, global health and the overuse of antibiotics and pesticides are all pressing issues that society and industry need to address in the need to shape a more sustainable future. At Chr. Hansen, we are positioned to drive positive change and addressing these challenges through our sustainable microbial solutions. Department of Chemical and Biochemical Engineering is, as a close partner, uniquely situated to provide innovative solutions and strong engineering candidates contributing to this essential purpose."



KATARINA LINDSTRÖM EXECUTIVE VICE PRESIDENT AND COO HEMPEL A/S

"At Hempel, our purpose is to shape a brighter future with sustainable coating solutions. Across the globe, our paints and coatings protect and beautify buildings, ships, infrastructure, and other assets, lowering their impact on the environment and enhancing their performance. Our strategy to double in size by 2025 makes our commitment to sustainability even more important. We have set ambitious science-based targets to reduce 90% emissions from our own operations by 2026 and 50% from our value chain by 2030. DTU Chemical Engineering is an invaluable partner for us to tap into the latest research, within the fields of formulations, processes, and sustainability. Cooperating with DTU Chemical Engineering also creates an excellent opportunity for attracting talent and developing future and existing Hempel employees."



CARSTEN RIISBERG LUND BOARD MEMBER, FORMER GROUP EXECUTIVE VICE PRESIDENT FLSMIDTH A/S

"The world must come together to solve the urgent challenges of global warming and scarcity of resources. Developing and commercializing practical technologies together is the hallmark of Danish industry and research institutions. DTU Chemical Engineering has for decades worked with Industrial partners to support and develop this hallmark on a local and global scale.

A unique technology position and strong engineering competences are the foundation for success for all process engineering companies that I am affiliated with. Through state-of-the-art education of international engineers, DTU Chemical Engineering shall continue to ensure the competence needed to maintain this foundation and together with industry we shall address the UN Sustainability Goals and develop practical and sustainable technologies applicable in the world at large."



MICHAEL HALLGREN SENIOR VICE PRESIDENT NOVO NORDISK A/S

"Kalundborg is the largest biomanufacturing hub in Scandinavia and an area in strong growth. From 2009 to 2019 it was Denmark's fastest growing municipality with an annual growth of 8.7% in GDP. Large investments have been attracted from both Danish and international companies. Since the turn of the millennium, Novo Nordisk has invested DKK 18 bn in the city - and recently we announced plans to invest DKK 18 bn. Establishing a world-class education and research environment targeted at the needs of the local industry will support continued growth in the region. Therefore, Novo Nordisk looks forward to collaborating with DTU Chemical Engineering on establishment of a MSc. in biomanufacturing in Kalundborg. With this initiative, DTU Chemical Engineering will contribute to further development in Kalundborg and in the region and support the future need for highly qualified labor."

# Teaching

KT considers research based and industrial inspired education and teaching our most important contribution to society and we are involved in:

- The BEng programmes "Chemical and Biochemical Engineering" and "Chemical Engineering and International Business".
- The BSc programmes in "Kemi og Teknologi", "General Engineering", and a new digital education taught in Danish, KT are contributing with the specialization in Power-to-X.
- The MSc programmes in "Advanced and Applied Chemistry", "Chemical and Biochemical Engineering", "Sustainable

Energy" (with special focus on Bio-Energy), as well as the N5TPolymers MSc programme. MSc in Chemical and Biochemical Engineering, Study line in Biomanufacturing (Industry MSc in Engineering, Kalundborg), and finally a Sino-Danish Master of Science programme in Chemical and Biochemical Engineering.

Our students work both theoretically and experimentally with the core disciplines in chemical engineering such as unit operations, transport phenomena, reaction engineering, mathematical modelling, and thermodynamics. They are taught by faculty specializing in these areas with applications in energy conversion, enzyme technology, and biotechnology, polymers, coating technology, catalysis, computer modeling, process and product design.

# Courses

### 1 SEPTEMBER 2022-31 AUGUST 2023

# **PHD COURSES**

28905	Advanced Topics in Process Systems Engineering
28908	Rheology of Complex Fluids (heavy)
28909	Thermodynamic Models, Fundamentals and Computational Aspects
28917	Statistical Thermondynamics for Chemical Engineering
28923	Uncertainty and Sensitivity Analysis of Numerical Models
28927	Advanced Topics in Process Technology
28928	Electrolyte Solution Thermodynamics
28930	Advances in Chemical and Biochemical
28932	Process Engineering Laboratory
28933	Introduction to Chemical Modification of Protein
	Therapeutics
28934	Automation and Control of Yeast Fermentation
28935	Fuel Characterization, Ash and Deposit Formation,
	Corrosion in Utility Boilers

# SINO-DANISH CENTER (SDC) COURSES

88700	Industrial reaction engineering
88701	Transport processes
88703	Laboratory experiments
88704	Progress in research
88705	Process design-principles & methods
88706	Technology economic management and organization
	(TEMO)
88708	Green chemical engineering
88709	Fluidization and multiphase flow
88710	Combustion and high temperature processes
88711	Industrial bioreaction engineering
88713	Green Challenge
88715	Biorefinery
88716	Coating science and technology
88717	Research immersion
-	

# Courses

# MSC, BSC, AND BENG COURSES

Below, course numbers and names are shown for 2022-2023, with the number of students attending shown in brackets. Bachelor of Engineering courses are marked with a **(B)**. The other courses are Bachelor of Science courses, Master of Science courses, or common courses.

#### FALL SEMESTER

**28001** Introduction to Chemistry and Chemical Engineering (60) 28012 Chemical and Biochemical Process Engineering (71) (B) 28016 Mathematical models for chemical and biochemical systems (58) (B) **28020** Introduction to Chemical and Biochemical Engineering (53) **28022** Unit Operations of Chemical Engineering and Biotechnology (70) **(B)** 28121 Chemical Unit Operations Laboratory (26) 28125 Chemical Unit Operations Laboratory (7) **28140** Introduction to Chemical Reaction Engineering (37) **28150** Introduction to Process Control (32) 28157 Process Design (32) (B) 28213 Polymer Technology (34) **28233** Recovery and Purification of Biological Products (115) 28242 Chemical Kinetics and Catalysis (39) **28244** Combustion and High Temperature Process (70) **28310** Chemical and Biochemical Product Design (45) 28315 Colloid and Surface Chemistry (35) **28316** Laboratory Course in Colloid and Surface Chemistry (11) 28322 Chemical Engineering Thermodynamics (53) (B) 28342 Chemical Reaction Engineering (41) (B) 28344 Biotechnology and Process Design (31) (B) 28352 Chemical Process Control (32) (B) 28420 Separation Processes (57) 28455 Process adaptation in fermentation based biomanufacturing (62) 28480 Biobusiness and Process Innovation (171) 28515 Enhanced Oil Recovery (12) **28530** Transport Processes (51) 28831 Computational Fluid Dynamics in Chemical Engineering (13) 28845 Chemical Reaction Engineering Laboratory (22) 28852 GMP og kvalitet i farmaceutisk, biotek og fødevareindustri praktisk version **28864** Introduction to Matlab Programming (14) 28870 Energy and Sustainability (133) 28872 Biorefinery (58)

# COURSES GIVEN IN CO-OPERATION WITH OTHER DEPARTMENTS:

23522	Rheology of Food and Biological Materials (18)	
26010	Introductory Project in Chemistry (48)	

**41686** Materials Science (27) **(B)** 

#### SPRING SEMESTER

	Mathematical Models for Chemical and Biochemical systems (34) <b>(B)</b>
28020	Introduction to Chemical and Biochemical Engineering (52)
28022	Unit Operations of Chemical Engineering and Biotechnology (25) (B)
28025	Bio Process Technology (32)
28121	Chemical Unit Operations Laboratory (15)
28157	Process Design (36) <b>(B)</b>
28160	Mathematical Models for Chemical Systems (30)
28212	Polymer Chemistry (47)
28214	Polymer Synthesis and Characterization (14)
28216	Organics Coatings Science and Technology (9)
28221	Chemical Engineering Thermodynamics (15)
28271	Thermal gasification and sustainability (13)
28322	Chemical Engineering Thermodynamics (26) (B)
28342	Chemical Reaction Engineering (65) (B)
28344	Biotechnology and Process Design (34) (B)
28345	Industrial BioReaction Engineering (86)
28346	Advanced fermentation technology practicum (18)
28350	Process Design: Principles and Methods (57)
28352	Chemical Process Control (29) <b>(B)</b>
28361	Chemical Engineering Model Analysis (65)
28415	Oil and Gas Production (7)
28423	Phase Equilibria for Separation Processes (26)
28434	Membrane Technology (49)
28443	Industrial Reaction Engineering (44)
28451	Optimizing Plantwide Control (33)
28535	Rheology of Complex Fluids (light) (1)
28850	Quality by Design (QbD): Integration of Product and Process
	Development (118)
28855	Good Manufactoring Practice (114)
28864	Introduction to Matlab Programming (37)
28871	Production of Biofuels (31)
28885	Technology and Economy of Oil and Gas Production (11) (B

#### COURSE GIVEN IN CO-OPERATION WITH OTHER DEPARTMENT

- **12701** Introduction to Living Systems (77)
- **26317** Instrumental Chemical Analysis (43)
- **27455** Microbial adaptation to industrial processes (84)
- 41686 Materials Science (59) (B)
- 41687 Exercises in Materials Science (16)

# **BACHELOR OF ENGINEERING DEGREES**

43 students finished their research programme for the BEng degree. The project titles are listed below:

Adaptive laboratory evolution for enhancing the tolerance to products in Actinobacillus succinogenes - Anne-Mette Haupt Houlby Ammonia dosing system with improved capacity and stability - Zilan Walid Alloush Determination of release rates from transdermal patches - Yasmin Salskov Nielsen Bioethanol upgrade: Fuel-to-pharma - Juliane Refsgaard Seeberg Mixing and transport of salt powders - Sebastian Eilertsen Sommer Cokes species in deactivated MTH catalysts - Cecilie Lotte Ljungberg Andersen Definition of sterilization and assembly of critical format parts in a grade A filling isolator - Maja Andersen Effect of modified lignin in high performance anticorrosive coatings - Amina Mirza Experimental solubility analysis of advanced solvents for CO2 capture - Maja Bojsen Thyme Experimental investigation of the fluid dynamic conditions in a mixing tank with help of PIV - Camilla Tue Baastrup Experimental investigation of the scale up of a chemical synthesis process - Mikkel Bay Florin Electrochemical characterization of state-of-the-art solid oxide electrolysis cells at industrially relevant conditions - Julie Hanne Kurtz Energy saving from using the OXxOFF equipment on Havnsø treatment plant - Frederik Pastoft Nielsen Removal of biogas impurities using P2X technologies - Michelle Cecilie Topsøe-Jensen and Isabella Blaabjerg Lund Gasification of textile wastes in a fluidized bed - Marco Møller Kristensen and Nicolai Elm Mold deposit tooling for injection moulding - Tobias Damgaard Salling Green, high performance technology for downsteam processing: Fouling during purification of succinic acid fermentation broth - Wai Fung Hui Inhibitive effect of chemically modified lignin in anti-corrosion coatings - Fatima Abdillahi Ismail Intumescent geopolymer coatings for fire protection of steel - Esma Nur Colak Study of kaolinitic clay calcination in different reactors - Nasro Hussein Hassan Ali Kinetic characterization study on syngas co-fermentation - Huzaifa Saeed Comparative study on methods for the extraction and characterization of polycyclic aromatic hydrocarbon (PAH) contaminants in biochars, using soxhlet extraction - Asmarah Igbal Microalgal cultivation for valorization of fishery wastewater using a litre scale photobioreactor - Oguzhan Erarslan Model-based capacity analysis and facility design - Sayed Rahman Gulabzoi and Sofie Hong Yu Grøndal Modelling of a microfiltration process - Mads Hyre-Jensen Monitoring of SIP (steam-in-place) - Validation process - Mark Peter Andersen Measurement of physical properties for solvents in CO<sub>2</sub> capture - Julie Talevska Poulsen Optimization of waste handling in a large-scale chemical production, with an environmental and economical perspective - Malte Rotne Hansen Optimization of deaeration from evaporators and preheaters - Wingny Zhuo Optimizing the deglycosylation step of a downstream process - Amenah Rachid Chehade Optimization of fermentate pretreatment using LUMiSizer analyzer - Jakob Jermiin Lerkenfeldt Frost Optimization of reverse osmosis membrane operation using a machine learning approach - Patrick Helmenkamp Achen Optimization of packing of a chromatographic process - Sarah Cetti Process optimization of pigment production in Talaromyces atroroseus - Sallie Bay Bonfils Process optimization for green energy production from Pressure Retarded Osmosis (PRO): The effect of water composition and fouling on the membrane performance - Tobias Senika Christensen Pure component data estimation and modelling of contaminant removal from vegetable oil via short-path distillation - Kristine Dang Drevsen Test and comparison of a new type of UF-membranes to current UF-membranes used by Novo Nordisk in their purification facilities - Theis Svane Kruse Development of dashboards (Tableau) for analysis of operations - Anders Broksø Letting and Magnus Adelsten Olsen The investigations of sustainable materials for catheter production - Camilla Zacho Larsen

# **BACHELOR OF SCIENCE DEGREES**

26 students finished their research programme for the BSc degree. The project titles are listed below:

Catalytic removal of N<sub>2</sub>O from ship flue gas using ammonia as fuel - **Mathilde Munch Jensen and Kira Trier Wang** Kinetic and spectroscopic investigations of catalytic reduction of N<sub>2</sub>O with NH<sub>3</sub> over a metal substituted zeolite - **Jens Christian Manniche** Kinetic and spectroscopic investigations of N<sub>2</sub>O decomposition over an Fe-zeolite catalyst - **Julie Primdal Toft** Modeling of stripping, absorption and reactions involving gases - **Caroline Grunnet Rudbeck** Conversion of syngas to light olefins over combined high temperature methanol synthesis and zeolite catalysts - **Louise Dybdal Nilsson** Towards sustainable stone wool production process: removal of sulfur from recycled materials - **Oliver Sebastian Mole and Sofie Ertel** Studies of the interplay between carrier effects and the catalytic reaction in CO<sub>2</sub> hydrogenation to methanol - **Jakob Lykke Fischer** Investigation of the hydrogen dependence in catalytic ammonia synthesis - **Kasper Jørgensen** Identification of intermediates in iron-catalyzed amoonia synthesis - **Aske Hansen** Effect of curing agents on the performance of lignin-based anticorrosive coatings - **Frederik Nikolaj Larsen** Experimental analysis of potassium - based Carbon Capture coupled with electrochemical regeneration - **Melissa Fernanda Rugholm Jensen** Impact of gas composition on syngas biomethanation - **Camilla Borregaard Thestrup** The influence of test conditions on intumescent particles for fire protective intumescent coatings - **Valdemar Willendrup**  Influence of hydrogen on the dynamics of catalytic methanol synthesis - Johanne Lønborg Christensen Conversion of CO<sub>2</sub> to light olefins over combined high temperature methanol synthesis and zeolite catalysts - Klara Jordahn Conversion of CO<sub>2</sub> to medium chain olefins and gasoline range hydrocarbons over combined high temperature methanol synthesis and zeolite catalysts - Janie Dittmann Weimar Andersen Formulation of biochar briquettes - Jens Aksel Rasch Madsen High-temperature oxidation of HNCO - Cecilie Kjærsgaard Juhl

PAT technologies in fermentation - Sara Hunding

Polymerization conducted under microwave irradiation - Peter Tang

Semi-continuous distillation - Sebastian Due

Thermal decomposition of N2O - Alexander Bonde Skov

Investigation of a phase separation device in pharmaceutical production - Nikolaj Sams Falkenberg

Investigation of the influence of foaming parameters on silicone foam performance for wound care - Mikkel Stub Neubert

# **MASTER OF SCIENCE DEGREES**

100 students finished their research projects for the MSc degree. The project titles are listed below::

Allergen protein capture by integrated particle sedimentation and ion exchange - David Lang and Anders Martin lensen Investigation of silica precipitation in a geothermal production process - Hulda Kristin Helgadóttir Advanced process understading of industrial fermentation - Camilo Andres Amaya Chica Benchmark analysis and optimization of renewable chemicals production - Bjarni Kristinn Bjarnason Carbon capture from biogas using innovative solvents: Modelling and experiments - Xenia Bonnén Sjøgren and Rasmus Juel Friis Data-driven control strategy for dewatering of inactivated biosolids - Alex Pokhrel Downstream process optimization and characterization of enzymes - Sara Grini Nielsen Dynamic supply planning - Miguel Carcas López Effect of bubble size on oxygen transfer - Emilie Overgaard Willer Electrochemical CO<sub>2</sub> pilot measurements and model - **Póra Kristín Jónsdóttir** A data-driven, modelling and simulation approach for an environmentally sustainable API capacity increase - Andreas Skovhøj Henriksen A generic biomass monitoring strategy for yeast cultivations in pilot scale - Marina Macedo Weber A robust approach to planning and decision support in a pharmaceutical manufacturing - Rune Christian Dates Andreasen A simulation model for bio-manufacturing process development and analysis - Pol Ubach Mases A stochastic approach for operational readiness in API pharmaceutical manufacturing - Rikke Vilsøe Nielsen Enzymatic hydrolysis of coffee oil - Paloma Sandra Rozene Vallespin A cyberphysical inspired design of an API pilot facility - Bertil Donsted Engberg Hybrid modeling of fermentation for the production of succinic acid by Actinobacillus succinogenes - Konstantinos Kiousis Fermentation optimization of a baking enzyme from Aspergillus oryzae - Martyna Joanna Piwowarczyk Generalized modelling of a soft sensor for an aerated bioreactor, based on multiple cell cultures - Frederik Nikolai Seehausen Knudsen Curing mechanism and curing kinetics of alkoxysilane curing paints - Matùs Kalina Impact of renewable fuels on particulate filters - Angel Hurtado Gozalo Industrial Symbiosis Design and Analysis - Guilherme Esteves Oliveira Frizado INOSIM capacity modelling and debottlenecking of large-scale fermentation plant - Marcus Koefoed Schnügger Characterization and optimization of hGH production - Rasmus Worre Beuchert Conceptual design of a stem cell therapy production facility - Nil Puig Engel Continuous chromatography - Magnus Lykke Poulsen Continuous separation of APIs - Amanda Skak Quantifying biomass sedimentation properties for improved centrifugation performance - Teodor Manne de Val Weywadt Quantifying bioreactor dynamics for identifying possible process improvements - Cristina Hotea Membrane modification for green energy production from Pressure Retarded Osmosis Technology (PRO): mechanical stability and the effect of temperature on the performance - Martin Flaskjær Buhl Model-based capacity analysis of synthetic peptide production in CMC API Pilots - Frederik Skovgaard Vogel and Christian Kirketerp Jacobsen Model Discrimination for Prediction of Dissolved CO2 profiles in CHO cell cultivation - Nikolaos Stefanidis Modelling of coagulation factor IX production in a perfusion bioreactor - Anna Oliver Almirall Modeling of mechanical properties of concatenated ring networks - Aliz Hanga Lelik Modelling and control of aeration and mixing time in fermentation reactors - Magnus Christian Holm Experimental and modelling of physical chemical CO<sub>2</sub> capture solvent properties - Simon Hjort Munk Downstream process design for the production of novel proteins - Claudia Brotons De Juan In-situ NOx Control in WtE Plants - Minh-Thao Pham Building cell-like structures by polyelectrolyte modification of polymer membranes: Improved enzyme immobilization and fouling performance - Jonas Sterup Brigsted Optimization of an industrial granulation process using dynamic image analysis - Andreas Würtz Optimization of an industrial, reactive crystallization process using design of experiments and process analytical technologies - Louise Riising Bentsen and Wania Saif

Optimizing protein and biomass yield by submerged fermentation of *Aspergillus oryzae* from beet molasses as main carbon source - Ivan Horacio Rosano Gazca

Optimization of Sn-Beta catalyst regeneration via kinetic modeling - Simon Rose Petersen High pressure oxidation of ammonia/hydrogen mixtures - Ivan Krstevski Para and meta separations - Joachim Herlevsen Comparison of enzyme immobilization strategies: PE-based support in enzymatic membrane reactor (MBR) and encapsulation in Metal Organic Framework (MOF) structures - Markus Simon De Martini Periodic stripping. Digital Twin - Lise Marijati Kjær Larsen Pigment recovery from fermentation broth - Søren Hornum Opstrup Use of pressure-retarded osmosis for production of green power: Experimental and modelling approaches for high membrane performance **Thomas Marschall Thostrup** Biopolymers processed and used as enzyme carrier - Dániel Mészáros Rational scale-down design & validation from compartment model simulations - Jean Victor Orth Study of dynamic instabilities in exothermic converters - Emil Daniel VBoman Bogan and Jacob Hyldgaard Rasmussen Techno-economic comparison of catalytic and biological PtX pathways - Julie Finne-Ipsen Techno-economic analysis and Process optimization of a legacy downstream process - Christian Venbierg Separation Process - Digital Shadow Development - Mathias Otto Barington Development of heterogeneous catalysts for hydrous cracking of glucose into glycolaldehyde - Maja Liv Hougaard Vester Development of syngas biomethanation process in trickle bed reactors - Eirini Thanasoula Water whitening in transparent antifouling coatings: Characterization and solutions - Kaare Halskov Anholm Investigation of variation in filterability of a high-concentration modern insulin drug product - Josu Arano Noriega Validation and adaption of heat transfer models in intumescent coatings - Ian Bartlomiej Krzak Understanding the adhesion of waterborne primers for high surface tolerance - Sofie Ye Lovmand Roedsted Alternative pasteurization method for breweries - Laurits Sehested Hansen At-line enzyme concentration measurements - Maria Alejandra Piza Bermudez Experimental investigation of novel solvents for CO<sub>2</sub> capture - Can Demir Performance evaluations of conformed catalysts for N<sub>2</sub>O abatement - Amanda Louise Petersen Understanding the response of glucose-sensitive transcription factors in E.coli - Yashomangalam Dinesh Bhutada Advancing Fermentation Process Monitoring: Integrated Glucose Monitoring via Innovative Electrochemical Sensors and Advanced Soft Sensor Technologies - Marc Lemperle In-line measurement of sugars in HMO fermentation - Katrine Lund Andersen Superior antifouling coatings for grooming technologies - Friderika Dora Varga Real-time characterization of batch precipitation and crystallization in downstream operations - Victoria Sara Saad Stability studies of benzoyl peroxide containing skincare products - Virginia Celestre Exchange of ceramic membrane filter unit - Mahmoud Samir Bayragdar Development of a full-valorization concept for selected effluents from the tanning industry - Karen Marker Investigation of the catalytic ammonia synthesis through microkinetic modeling - Malene Stryhn Thestrup Jensen Kinetic measurements of CO<sub>2</sub> reactivity with innovative capture solvents - Simone Skaale Christoffersen Development and deployment of Deep-learning based property models - Alessandro Cogliati Effect of electron donors in Syngas Fermentation - Iulian-Gabriel Alexe Establishment of microbial cell factories tolerant to lignocellulosic hydrolysate - Joaquín Jacobo Ucha Gavilán Establishing and scaling a continuous fermentation process for atrorosins production by Talaromyces atroroseus - Sergio Fuentes Liso Gel-life time monitoring and optimization of chromatography columns in industrial pharmaceutical manufacturing - Pablo Sanchez Nieves Feasibility and viability of regeneration and re-use of CIP chemicals - Yujing Zhao High throughput, high capacity membranes for bioseparations - Otilia Tatiana Marc Implementation of an innovative power plant: Case study of an osmotic energy plant - Violette Suzanne Jacqueline Isoré Integration of Bioelectrochemical Systems in a Syngas Fermentation Process - Pantelis Bountzis Mathematical modelling, control strategies and optimization of an ultrafiltration process for protein powder production - Zsolt Kovacs Membrane recovery of human serum albumin from P. pastoris - Daniel Nymand Petersen Modelling the water recovery from waste water treatment systems with Machine Learning - Rasmus Nissen Dahl Milk without cows - are there sustainable alternatives? - Benjamin Thomas Aust Optimization of image analysis crystal classification using machine learning and process analytical technologies - Helena Haarup Lauritzen Reinforcement learning for statistical process control in API manufacturing - Tanish Dhagat Systematic development of mechanistic models for industrial fed-batch fermentation processes - Caroline Hamelmann Techno-economic analysis of a solar ammonia and fertilizer production - Pablo Lopez Martinez Developing a tailormade software alternative for mass balance reconciliation in the fermentation section of an API manufacturing facility -**Carlota Faus Ferrer** 

Effect of antifoam on CHO cell culture aeration - Josephine Marie Levin Patheier

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# PhD thesis defences **2023**

### **Evangelos Tsochantaris**

Advanced Thermodynamic Models for Water

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