Annual Solution of the second second



Tenna Frydenberg (Industrial PhD student at EnCoat ApS and CoaST Research centre, DTU Chemical Engineering) testing the performance of more environment-friendly and sustainable antifouling coatings at CoaST Maritime Test Centre at the Port of Hundested.

Dorte V.P. Sommer

Contents

04	Welcome
06	Key numbers
80	Keep your microorganism happy
12	The Pilot Plant goes digital
15	Sustainable chemistry through new software
18	Introducing e-plastic
22	A larger role for chemistry in polymer recycling
25	Microalgae valorize potato starch by-product
28	Give us fouling, please!
32	Carbon capture by alkali absorption
36	Highlights
42	Cooperating companies
43	A new KTStudents board
44	Organization
45	The Faculty
46	Teaching
52	Publications
62	PhD thesis defences

Changing the world with sustainable and digital solutions

The growing global demand for energy and resources and the problems of scarcity and environmental impact are some of the main challenges of the world.

At DTU Chemical Engineering, we believe that solutions must be found through science and engineering followed up by political actions if we are to limit the negative environmental and climate consequences of human behaviour. Therefore, developing technologies for sustainable change within our scientific fields has been a focal point at the Department for many years.

In this year's annual report, you can find examples of technical solutions supporting

sustainable change. One is a Danish-Dutch partnership that investigates a new approach for carbon capture using alkali absorption. Another is the activities in the Port of Hundested, where researchers are exposing painted samples to real-life conditions with the aim of developing anti-fouling coatings with improved sustainability properties.

Our focus is also on more recycling and reutilization. For example, we have several projects exploring different ways of recycling polymers using and optimizing different techniques based on both chemical and biological methods. Other researchers show how to turn low-value waste streams from production of potato starch into high-value products.





Realizing the opportunities of digitalization in chemical and biochemical engineering is another focal point. From the beginning of 2022, students, researchers, and industry users can train virtually, remotely, or on location, before starting their experiments at our Pilot Plant, making the Pilot Plant more accessible to a wider range of users. Utilizing the many digital opportunities is also evident with a new virtual laboratory under development at the Department. The lab provides students with the opportunity to study optimization of industrial processes virtually, and is a great supplement to the physical lab education.

Creating new ways for training purposes is one way we seek to create value-adding technology for people. Another is through developing new tools to help industry progress with their sustainable developments. For example, a new software tool, developed at the Department, can help companies finding the best ionic liquids for specific applications.

As in 2020, Covid-19 played a significant role for our students, industrial and academic partners and employees. However, despite the pandemic and the many challenges it brought on, 2021 was a good year for DTU Chemical Engineering.

Educating and preparing the next generation of chemical engineers for future challenges is one of our most significant contributions to society. Again, we saw a high number of students at our courses, and our study line in Fermentation Based Biomanufacturing was well received.

We have gained, but also lost great employees the past year. I would particularly like to highlight that we in January 2021, welcomed a new research group to the Department, headed by Professor Irini Angelidaki. The new Bioconversions group is a great addition to the area of microorganisms and how these can be used as tools to transform organic waste and wastewater into useful products. Sadly, in July, Professor Emeritus John Villadsen passed away, and we lost a great and inspiring chemical engineer, and a good friend.

Looking ahead, we are optimistic. We have strong collaborations with industry, we see a bright generation of future chemical engineers making their mark on the world, and we have skilled and dedicated employees at the Department. This is a position we do not take for granted, but we will do our very best to keep contributing to finding new solutions for the benefit of society.

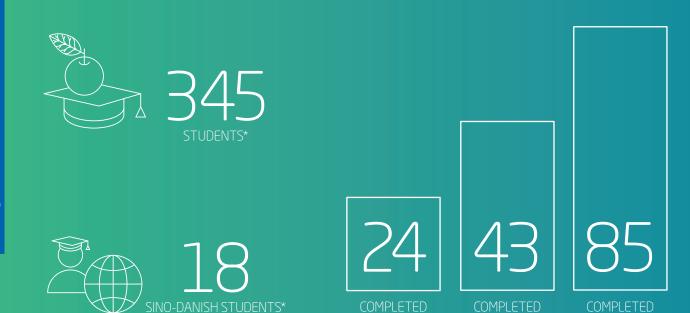
Kim Dam-Johansen Professor, Head of Department



Kim Dam-Johansen Professor, Head of Department



EDUCATION



RESEARCH



246 SCIENTIFIC ARTICLES IN VOS-INDEXED JOURNALS









INNOVATION



ORGANIZATION













63 RESEARCHERS / SENIOR RESEARCHERS



PHD STUDENTS (INCLUDING 10 INDUSTRIAL PHD'S)

Keep your microorganism happy

A new Virtual Laboratory at DTU Chemical Engineering allows studying optimization of industrial bioprocesses.

Yeast, bacteria, and other microorganisms play the leading roles in a newly developed Virtual Laboratory at the Department. The lab has been developed with an educational goal with students as the primary target group.

"As chemical engineers, we have simulated traditional industrial processes for decades. Simulation of biological processes has been challenging, but since industry moves more and more into bioengineering, the value of being able to simulate bioprocesses has become apparent," says PhD Researcher Simoneta Caño de las Heras, PROSYS, DTU Chemical Engineering. She has developed the virtual lab in her PhD project 'Development of a Virtual Educational Bioprocess Plant'.

In its core, simulation of bioprocesses is not that different from other chemical engineering simulations, Simoneta Caño explains:

"For the most frequently used microorganisms in industry, we do have relatively reliable models. We know that if a given organism is subjected to a given temperature and level of nutrition etc., its growth can be projected mathematically. And when you can describe your system mathematically, you will also be able to optimize."

However, some features do make simulation of bioprocesses extra challenging:

"Microorganisms are alive. You may not necessarily see any dramatic events, but if the microorganisms are not "happy", production will not be optimal."

Developed by students for students

The lab is a virtual bioprocessing plant. A typical task might be to calculate the necessary volume and height of a bioreactor for a given purpose.

"We realized that our students simply need to have knowledge in this field. Optimization of bioprocesses does not only improve business cases in industry, but also contributes to making production more sustainable by minimizing the consumption of energy and other resources," says Associate Professor Ulrich Krühne, supervising the project.

He adds that the primary goal is educational:

"The problems to be solved in the virtual lab are all relevant in an industrial context, and possibly some companies may be able to benefit from using the lab, but first and foremost it is a tool for students—and made by students," notes Ulrich Krühne.

Using the lab does require knowledge of bioprocesses, Simoneta Caño underlines:

"Both bachelor and master students here at DTU will surely find the tool useful. The same goes for technicians operating bioprocessing facilities. Also, for instance a high school student wanting to explore the combination of biology and math as a possible future career path would be served well."





Coding experience required

Further, users will need to have basic coding experience. This is a deliberate choice, according to Simoneta Caño:

"Industrial bioprocessing is a field in rapid development. Therefore, we wanted to make it possible to enter new organisms, new processes, and new parameters."

Coding is in PYTHON. Users may choose either easy, medium, or hard.

"When we tested the first version of the lab, some students complained about the tool being too easy, as they noted industry would expect them to have more advanced coding experience. Therefore, we decided to provide three different levels," says Simoneta Caño, continuing:

"Further, we have included coding exercises to encourage independent thinking. Some exercises have deliberate errors here and there, and the task is to find these errors. And sometimes the virtual laboratory will propose unfeasible scenarios while challenging the user to discover the problem. We want especially students to constantly consider what they are doing, not just have our software do all the work for them." The virtual lab is already being used by DTU bachelor students. It is available at www. biovl.com.

Whether training in the virtual lab should be included formally in bachelor and/or master education is yet to be decided.

Contributes to sustainable solutions

Students will not be able to skip their hours in the physical labs just because they have access to a virtual one:

"The virtual lab cannot substitute for lab experiments. Instead, the virtual lab is a complementary tool which will help the students raise the quality of their experiments. In this way, the project is a part of the new trend of blending physical and virtual education," notes Simoneta Caño.

She adds that considering the large societal benefits from better bioprocesses, it was decided that the lab should be openly accessible and free of charge:

"This is a case of a public institution being able to contribute to more sustainable solutions. Further, we have created a tool that will not only benefit the students at DTU and other Danish universities. Just to take an example, South Africa is currently seeing a boom in bioprocessing. Bioprocessing innovators may not be able to pay for commercial simulators, especially not in developing countries. A tool like this, has a potential for making a difference in many places."

New project will add artificial intelligence

In her project, Simoneta Caño has built the virtual lab all the way from the basic handwritten stoichiometric table on microbial growth over models to the graphic user interfaces. On the path to complete her PhD degree, she leaves DTU to work in biotech industry. Responsible for maintenance and further development of the virtual lab will be Fiammetta Caccavale who commences a new PhD project. Here, some artificial intelligence (AI) tools will be added. The AI will note the main interests of individual students, and thereby allow for personalized learning.

"To our knowledge, the lab could become the first biochemical engineering tool with built-in artificial intelligence," says Simoneta Caño rounding off with a smile:

"During the last three years, I have become very connected to the virtual lab, but I am sure Fiammetta Caccavale will take good care of my "baby"!".

- Simoneta Caño de las Heras, PhD Researcher
- Ulrich Krühne, Associate Professor

Process and Systems Engineering Centre

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 supporting 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, including also the 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 development/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), 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 is involved in a broad range of industry collaborations. At the Department, we have frequent collaborations with PILOT.

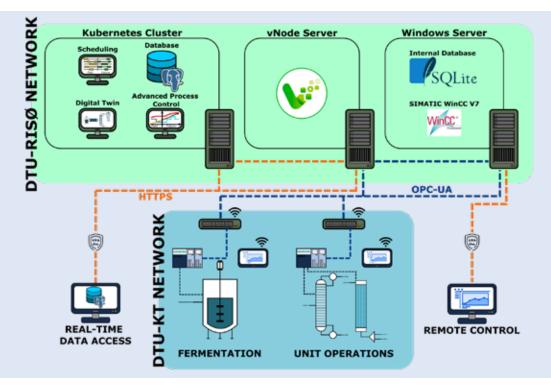
The Pilot Plant goes digital

Researchers, students, and industrial users will from now on be able to hit the ground running, when starting experiments at the Department's Pilot Plant.

Students, researchers, and industry users can as of 1 January 2022, train virtually before they start experiments at the Pilot Plant at DTU Chemical Engineering.

"We always emphasize that our users need to prepare beforehand, as they otherwise risk wasting valuable time until they become acquainted with our units. From now on they can do this preparation in a virtual version of the equipment," says Steen Larsen, Head of Pilot Plant. Having downloaded the relevant software, the user will be able to train either remotely or on location. The user enters a virtual representation of the actual Pilot Plant main hall. Six facilities in the hall are accessible for virtual operation, and more will follow.

It should be stressed that the virtual operation of the equipment is for training purposes only. It is not yet possible to operate the real equipment from a distance, nor to conduct simulated experiments.



Scheme of the Pilot 4.0 infrastructure for supervisory control and data acquisition (SCADA) and data storage in the relational PostgreSQL database. Mads Stevnsborg

"The value lies in our users getting a feeling for operating the unit before they come here to start the experiment. Where are the various handles for valves, pumps etc.? How are they operated, and in which order? Most users find the virtual operation much more appealing than reading a manual," explains Steen Larsen.

Makes the Pilot Plant more accessible

In a wider perspective, the virtual product contributes to making the Pilot Plant more accessible, notes Steen Larsen:

"The equipment here constitutes a very large asset. Until now it has mainly been used for educational purposes, but we are confident it can be used more in research than today. Also, while we do have industrial users, mainly from SME's and startup companies, we hope to welcome more."

The virtual Pilot Plant is just the tip of a larger iceberg when it comes to digitalization.

"The data produced during operation of the units at the Pilot Plant have a value beyond the individual experiment. Maybe in, say, six years' time another experiment in the same field can benefit from an experiment conducted today. However, this additional value can only be harvested if we are able to arrange data collection and storage in a systematic manner and secure future access to the meta data," explains Postdoc Jochen Dreyer, responsible for the SCADA (Supervisory Control and Data Acquisition) implementation at Pilot Plant.

Balancing systematics versus flexibility

Systematic data collection and storage at an experimental facility is harder than it sounds, Jochen Dreyer elaborates:

"While an industrial facility will run the same process continuously, our users will typically run shorter projects or exercises for maybe five-six hours and may even change process conditions along the way. This makes systematic data collection highly challenging. If we set rigid demands for the data collection, we will not be able to capture the creative ideas, but if we let people completely loose, we will end up with a messy database that cannot be used later. So, it's about finding a compromise between keeping things systematic versus flexible. It has taken a lot of effort to strike the right balance."

Steen Larsen joins in:

"When researchers come here, they can work on their research and do not need to think about data collection. Still, considering the rapid development within automation and digitalization, I would not dare to say that we have found the optimal solution. I believe everybody's trying to find their way, and that goes for industry too."

The Pilot Plant has been able to benefit from other developments at DTU, notes Jochen Dreyer:

"We have been able to use server capacity at DTU Research-IT at Risø and tap into their expertise in server administration. This has allowed us to try out different setups and decide on the specification for our own servers."

Not striving for full automation

An underlying aim behind the virtual Pilot Plant is to introduce the DTU students to automation, Steen Larsen points out:

"Currently, all equipment at the Pilot Plant is operated manually, as we wanted our students to get a feeling for operating the valves and pumps during their experiments. Still, we must recognize that automation, web-based user interfaces, control systems and Big Data are an increasing part of the industrial reality. While we are not striving for full automation, we need to let our students experience state-of-the-art automation."

Not surprisingly, users have welcomed the virtual Pilot Plant, according to Steen Larsen: "Especially the younger users would never come here with pen and paper, but rather work on their digital devices. Getting acquainted with the equipment through a virtual Pilot Plant is just very natural for them."

Steen Larsen, Head of Pilot Plant

실 Jochen Dreyer, Postdoc

Pilot Plant

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 was initiated in 2021, a project that will continue in the years to come. 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.

During 2022, we will add new manpower resources to increase our focus on research and innovation activities based on processes, technologies and equipment. This will create and enhance an even more dynamic interface and activity between our capabilities and the external collaborators.

A new pilot scale fermentation-based manufacturing line of pharmaceuticals, food, biochemicals, and biofuels, including biomass pretreatment, fermenters from lab scale-up to 300 litres and relevant downstream separation and purification equipment, will be approved for handling Genetically Modified Organisms (class 1) during the first part of 2022.

Sustainable chemistry through new software

lonic liquids hold a huge potential for improving energy efficiency and environmental friendliness of chemical engineering processes. A new software tool from KT Consortium will assist innovators in finding the best ionic liquids for specific applications.

lonic liquids are salts. However, unlike the common perception of salts, they are liquid at room temperature. Further, the vapour pressure in ionic liquids is extremely low, close to negligible. In numerous chemical engineering applications, this is a highly interesting property.

Some industries already have applied ionic liquids in their processes. Examples are NH₃ recovery, electrolytes, cellulose spinning, methyl methacrylate (MMA), iso-octane clean tech, and ethylene glycol/dimethyl carbonate (source: Industry of Process Engineering, Chinese Academy of Sciences). However, these examples may well be a modest beginning of a new era of chemical engineering applications with ionic liquids.

Carbon capture is one example of an important technology in need of more efficient and sustainable chemistry. Ionic liquids are a likely solution to the challenge. But how do you identify the best molecule for the job, when a huge number of different ionic liquids exist?

"It is just not possible to find the optimal ionic liquid molecule for a given task through traditional lab experiments. For this reason, we decided to develop a computational tool which may assist developers. The tool will not identify the ideal molecule, but it may screen many potential molecules, narrowing the field down," says Guoliang Wang, Software Manager at KT Consortium.

Based on a PhD project by Yuqiu Chen– currently Postdoc at DTU Chemical Engineering–supervised by Professors John M. Woodley and Georgios M. Kontogeorgis, Guoliang Wang has developed the new tool which is named IL Pro.

Vapour pressure close to zero

"If we take carbon capture as an example, some amounts of the amine-based solvents which are traditionally used will be lost due to evaporation. This adds to the costs and potentially leads to emissions. If instead, we can replace these solvents with an ionic liquid, the amounts of lost solvent will be close to zero while the energy-efficiency can be greatly improved," explains Associate Professor Xiaodong Liang, also a member of the project team.

Another potential application is in batteries. With increasing demands for electric cars, photo voltaic cells, wind power, and several other electric technologies, the need for more efficient and environmentally benign batteries is becoming still more urgent.

"Ionic liquids are promising as safe and energy-efficient alternatives to flammable organic solvents currently used for instance in Lithium batteries," notes Xiaodong Liang. Also, in fields like pharmaceuticals, waste recycling, catalysis, biopolymers, and other bioprocesses ionic liquids are likely to enter the scene.

Needle in haystack

Being salts, ionic liquids always consist of both a positively charged group, the cation, and a negatively charged group, the anion. Further, many side-groups can be attached to either ion. This can be translated into an enormous range of ionic liquids which could potentially be synthesized.

Theoretically, it is possible to synthesize 10¹⁸ different ionic liquids. The large number of candidates means that identifying the best one can seem like finding the needle in a hay-stack. This is the challenge faced by industry.

"Several KT Consortium member companies have expressed interest in ionic liquids and in software for assessment of ionic liquid applications," says Xiaodong Liang. He further notes that the interest was confirmed, as KT Consortium did a survey among industry participants at its annual meeting.

The 1.0 version of the IL Pro was launched in June 2021 and consists of a Database Manager and the IL ProPred. The latter tool is an ionic liquid focused version of the ProPred application from ICAS software (Integrated Computer Aided System) which is one of the main KT Consortium deliverables. The software combines computer-aided tools for modelling, simulation, property prediction, synthesis/design, control, and analysis. ProPred assists by predicting the properties of a new substance under consideration. In this way, developers may save time and costs by not synthesizing substances with suboptimal properties.

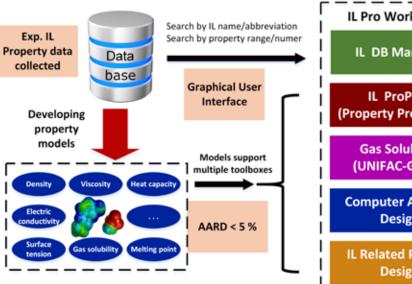
"We hope that the 1.0 version will be of assistance to our industry colleagues. Still, the tools in this version are only a first step, more functionalities will be added" says Guoliang Wang.

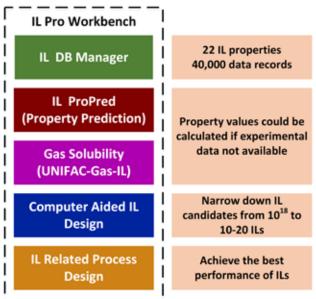
Artificial intelligence as a future step

The IL Pro version 2.0 is due to be launched in June 2022. Here, UNIFAC-IL-Gas extension models and a molecule design feature for lonic Liquids will be added. And in June 2023, the team plans to launch IL Pro version 3.0 with ionic liquid process design included.

"We have seen interest from industry already, but I expect the inclusion of process design will be the feature that really spurs wide interest," says Xiaodong Liang.

- 🛆 Guoliang Wang, Software Manager
- Xiaodong Liang, Associate Professor





KT Consortium

At KT Consortium we work on bringing together advances and developments made in the area of process systems engineering, bio-process engineering, applied thermodynamics and property prediction at DTU Chemical Engineering and to continuously improve and innovate for a better and more sustainable future.

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 DTU Chemical Engineering.

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:

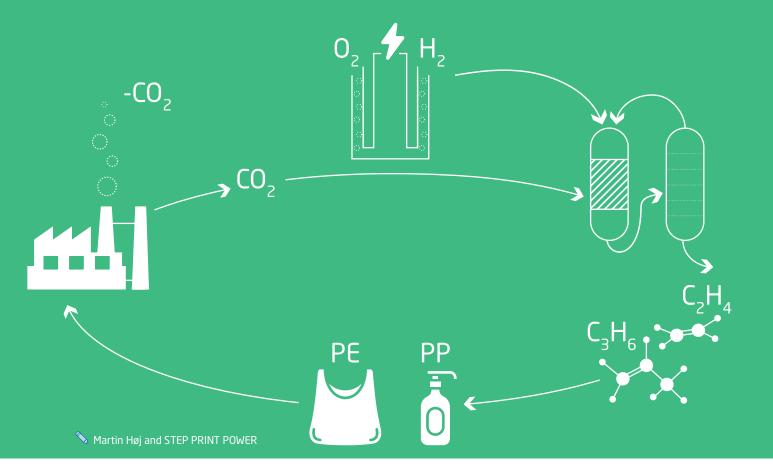
1. Participation in the Annual Meeting

- 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.



Introducing e-plastic

Many polymer waste fractions are hard to recycle mechanically. For these fractions, a relevant recycling technique could be incineration followed by CO_2 capture with the aim of manufacturing new polymer materials by reacting CO_2 with hydrogen (H₂). This is the focus of the project ' CO_2 to Monomers' at the CHEC research centre, DTU Chemical Engineering.

"Using CO₂ as a raw material for making new polymer building blocks is not in itself a new idea. Several industrial trials are already taking place. However, low economic costs will be crucial for the practical feasibility of the concept. Our ambition is to eliminate some of the steps of the current efforts. If we succeed in developing a onestep process, chances of minimizing costs will be good," explains Associate Professor Martin Høj, Project Manager.

The project develops a process for direct

conversion of CO₂ and H₂ into light olefins and/or aromatics as plastic monomers or monomer precursors. The CO₂ could be obtained by carbon capture from incineration of polymer waste fractions, which are difficult or overly costly to recycle. However, the CO₂ could also come from other sources, such as biomass gasification or biogas upgrading. The H₂ could be obtained from water electrolysis, where the power for the electrolysis should be renewable energy such a wind or solar power, possibly combined with biomass gasification. When using electrolytic hydrogen, the concept is sometimes referred to as e-plastic.

Products are high-value polymers

"The e-plastic concept is related to the concept of e-fuels and more broadly to Powerto-X. The idea of producing monomers from $CO_2/CO/H_2$ (syngas) mixtures dates back to the 1980'ies but has only gained momentum within the last three years or so, as Power-to-X has become the centre of attention," notes Martin Høj.

The idea is not to incinerate all polymer waste.

"For certain fractions, direct recycling is possible. However, 100 per cent polymer recycling by purely mechanical techniques can never be achieved. It will only be possible to keep the recycling going by adding some amount of pristine polymer while also removing some amount of the degraded polymer. This is where chemical recycling becomes relevant," comments Martin Høj.

E-plastic is a chemical recycling technique. The incineration results in CO_2 , which is then reacted with H_2 to form methanol (CH_3OH). The methanol can be further converted into olefins and/or aromatics as plastic monomers or precursors for monomers. "Here we see a big advantage of chemical recycling. The end product will be a high-value polymer, or virgin polymer if you like. It will not be possible to distinguish between a polymer produced in this way and a polymer produced for instance from fossil raw material. Both can act as the high-value polymer necessary for mechanical recycling of other polymer fractions," says Martin Høj.

Circumvents equilibrium limitation

"Admittedly, if an evaluation of the economic feasibility was to be carried out right now, it would point to e-plastic as very expensive. However, this would largely be because CO_2 can presently be emitted into the atmosphere at very low cost. As we are seeing upcoming demands for CO_2 capture and storage, the relative costs of making use of CO_2 as raw material are due to be reduced."

In current industrial trials, the processes will initially yield so-called syngas which is a mixture of CO₂, CO, and H₂. The syngas is then converted into methanol, which is later processed into monomers. In 'CO₂ to Monomers', methanol will also be formed but will only exist shortly in the reactor as the methanol will be reacted directly into the desired end products. Taking this short-cut is enabled by use of a tailor-made catalyst system.

Several projects on chemical polymer recycling

The incineration concept of the 'CO₂ to Monomers' project is not the only technique for chemical recycling of polymers. Another technique is pyrolysis. Here, plastic is cracked down to fractions of shorter carbon chains. The end product is a fluid which resembles petrol. The project 'Bi-cycle', headed by Professor Anker D. Jensen, investigates this technique. The two projects run in parallel. Both were initiated in autumn 2020, run for three years, and are financed by the Independent Research Fund Denmark, Technology and Production Sciences.

A third CHEC project, titled 'Reburn', addresses the energy aspect of polymer waste incineration. When polymer waste is incinerated to produce CO_2 for production of e-plastic, heat is also produced. This heat should obviously be exploited. Also, some issues regarding prophylactic measures to ensure a clean exhaust gas stream from this incineration needs to be addressed. The 'Reburn' project is coordinated by Associate Professor Hao Wu.

The projects on polymer recycling in CHEC are coordinated with another centre at DTU Chemical Engineering, the Danish Polymer Centre (DPC) (see article page 22, ed.).

"Besides the improved economy of having a direct process, another advantage is that we circumvent the equilibrium limitation related to the methanol synthesis. Thereby, we can achieve a higher yield of the desired end products," explains Martin Høj.

Still fundamental research

The goal of the three-year project is to achieve 80 per cent selectivity for production of olefins with 15 per cent conversion per catalytic cycle.

"We still have plenty of work to do. Producing our end products in a direct process involves several trade-offs. We need to manage the field of reactions and find a compromise which results in the best economic feasibility possible," notes Martin Høj. Haldor Topsøe A/S is involved in the project as industrial partner. However, this should not be seen as an indication of industrial implementation being just around the corner, Martin Høj underscores:

"After all, real efforts to develop e-plastic have just come about during the last three years, and what we are trying to create here is an entirely new, more direct pathway. The perspectives are huge since polymer waste is both a large societal challenge and a potentially valuable resource, but our approach should definitely still be seen as fundamental research."

Artin Høj, Associate Professor



The CHEC Research Centre

The CHEC Research Centre at DTU Chemical Engineering carries out research in fields related to chemical reaction engineering, with 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 production, heat and power production, transportation, and energy-intensive industry.

Important areas include Power-to-X technologies, development of carbon-free energy carriers such as ammonia or metals, use of alternative fuels such as biomass or waste for power and fuel production, micellar catalysis replacing conventional organic synthesis in fine chemicals production and emission control. CHEC has achieved international recognition through a combination of experiments and mathematical modelling, based on chemical kinetics, chemical reaction engineering, thermodynamics, gas phase spectroscopy, and fluid dynamics.

Laboratory reactors are used to characterize gas-phase, gas-solid, and catalysed reactions at atmospheric or high pressure in a wide range of temperatures, 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).

A larger role for chemistry in polymer recycling

In the ideal circular economy, a given waste material would be directly recycled for the same purpose again and again. However, this is not always possible in the case of polymers since for each cycle, the polymers lose some of their attractive properties or accumulate impurities that prohibit some applications. Therefore, a range of different techniques will be required to achieve close to 100 per cent recycling.

"We need to create a systematic approach to the field, ensuring that each fraction is treated in the manner which achieves the highest possible value from a given material source," says Anders E. Daugaard, Associate Professor with the Danish Polymer Centre (DPC) at DTU Chemical Engineering.

For many fractions, recycling is challenging either because different types of polymers are blended or because the polymers have become polluted through their use cycles.

"Depending on their purity, it would be too expensive to separate the stream and to even attempt to purify the materials from an economic as well as a resource point of view. This leaves us with a lower-quality material that cannot easily enter mechanical recycling. Instead, our approach will be to subject these tricky polymer fractions to chemical treatment to obtain value," Anders E. Daugaard explains.

Pyrolysis entering the stage

One interesting chemical technique is pyrolysis. Here, polymer waste is heated in an inert atmosphere, and a resulting combination of oil and gas can be obtained. The liquid product can either be processed into a liquid fuel or be used as raw material for new polymers. Employing various catalytic pathways to upgrade these fractions to higher value materials is the focus of another centre at DTU Chemical Engineering, CHEC (see article page 19, ed.), whereas exploiting the monomers or crude products directly takes place in DPC.

As for the high end of the recycling hierarchy where direct mechanical treatment is feasible, DPC is active in the project 'Circular' funded by Innovation Fund Denmark with several industrial partners.

As for the chemical techniques, DPC is leading a project named 'Replastic' in close collaboration with CHEC. This project is also funded by Innovation Fund Denmark.

"Especially pyrolysis is a fertile ground for innovations. We see a lot of movement in this field right now. It will be very interesting to follow these developments in the coming years, and to see which waste fractions will become available for pyrolysis and where the cut against mechanical recycling will stabilize. Especially, the degree of purity and requirement for pre-treatment will be crucial in establishing sustainable use of these waste fractions," says Anders E. Daugaard.

Design with an eye to recycling

The DPC researchers do not accept the current pattern of polymer waste fractions as predetermined:

"The materials we see as waste today have almost entirely been designed based on considerations over technical properties versus price. Hopefully, we will soon begin to see materials which have been designed with an eye to recycling. Our task is to contribute with candidate polymers."

As an example, Anders E. Daugaard points to modifications which may increase the mechanical and/or thermodynamic stability of a polymer for it to tolerate recycling better:

"Our aim is always to move a given waste fraction upwards in the recycling hierarchy. Every time we can achieve a more direct kind of recycling, we improve sustainability."

Another step in the same direction is avoiding materials which are hybrids of different polymer species:

"If a product contains both, say, PE and PP (polyethylene and polypropylene, two of the dominant commodity plastics, ed.), it is just very difficult to recycle. Often it will be possible to achieve the desired technical properties using only one of the two, but in a modified version."

Recycling of bioplastics still in its infancy Finally, new bio-based and potentially biodegradable materials coming to market will additionally complicate the potential recycling pathways. DPC is a partner in the EU project 'UPLIFT', coordinated by Aalborg University, where biological recycling methods and polymers produced from renewable feedstock are in focus.

"Our role in 'UPLIFT' is to suggest ways to make use of the chemical building blocks which result from recycling of bio-plastics. This field is still in its infancy. Current bioplastics have typically not been designed with an eye to recycling. On the contrary, they are meant to be composted or incinerated with food waste. However, we will undoubtedly see interest in recycling of bioplastics," says Anders E. Daugaard, summing up:

"Both mechanical, chemical, and biological methods will be necessary. They are not really in competition since polymer waste consists of many different fractions, and there is no shortage of raw materials. The amounts continue to grow rapidly, and we see a huge push from consumers, politicians, and industry to get better at recycling polymers in sustainable ways."

Anders E. Daugaard, Associate Professor

🙆 Christian O. Carlsson 📹

The Danish Polymer Centre

DPC

The Danish Polymer Centre aims at being at the forefront of 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 for the research area is to lead the way towards more sustainable materials. We aim to take part in the transition at all levels of materials development from fundamental synthesis of new biobased polymers, across various recycling pathways, and towards 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 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 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 an easier recycling and permits 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 leverage across a broad range of products both in collaboration with other academic institutions as well as with industry.

Microalgae valorize potato starch by-product

Research at DTU Chemical Engineering has demonstrated how a low-value side stream product from production of potato starch can be turned into high-value dietary supplements and cosmetics.

Besides the main product potato starch several side streams are produced at KMC (Kartoffelmelcentralen). One of them is the low-value fertilizer protamylasses. The Bioconversions group at DTU Chemical Engineering has successfully used protamylasses as medium for cultivation of the microalgae species Haematococcus pluvialis. The algae produce astaxanthin, a high-value substance. Astaxanthin is an antioxidant which may contribute to protect cells from damage, and possibly strengthen the human immune defence. Further, astaxanthin is used as dietary supplement for human consumption, as colour additive in cosmetics, and as feed additive for fish. Astaxanthin is the substance which gives salmon its reddish colour. The market value of astaxanthin ranges around EUR 2,500 per kilo.

"KMC is representative for the increasing trend to view bioeconomic production in a wider context. By focusing on a suite of products based on the same raw material, rather than a single product, the company becomes more resilient to market changes, while also minimizing waste and contributing to a circular economy," says Professor Irini Angelidaki, head of Bioconversions.

Better cultivation medium

In the PhD project of Minmin Pan, supervised by Irini Angelidaki, the group succeeded in cultivating *H. pluvialis* on protamylasses. This microalgae species was chosen exactly for its ability to produce astaxanthin. However, the cultivation was not straightforward. Not only do the algae need nutrients, they also depend on sunlight. Since the concentration of nutrients and organic particles is very high in protamylasses fluid, it soon becomes dark, resembling heavy oil, blocking the sunlight.

Therefore, the research team could not grow the microalgae directly, but had to reduce especially the organic carbon content to make the environment suitable.

Firstly, the protamylasses fluid was introduced to anaerobic digestion/fermentation bioreactors. Here, part of the organic matter was converted into biogas—another valuable product. This significantly improved the composition of the fluid as a medium for cultivation of *H. pluvialis*.

"The effluent from the anaerobic digestion steps still had high concentrations of ammonium, phosphate, and acetate, which was very advantageous for the growth of the algae. In fact, *H. pluvialis* was growing much better in this medium compared to the standard medium commonly used for cultivation of this microalgae species," explains Irini Angelidaki.

Potential for significant monetary value

Unexpectedly, promotion of astaxanthin was also achieved during the following induction phase.

"We attribute the improved astaxanthin production to the content of potassium and acetate, which presumably played a key role in the induction phase. Using the proposed integrated approach, we could significantly increase the production of astaxanthin, while minimizing the period of cultivation and induction duration," comments Irini Angelidaki.

Producing biogas and astaxanthin according to this scheme has potential for bringing significant monetary value to KMC. The company already has widened its product portfolio from potato starch to proteins and other valuable products, all produced from potato feedstock.

From bioenergy to a suite of products

The Bioconversions group currently consists of some 15 researchers. Recently, the group joined DTU Chemical Engineering and was reorganized.

"Previously, we were called Bioenergy and were part of another organization at DTU. That name reflected how renewable energy used to be the primary focus of bioconversion. In recent years however, other renewable energy forms such as wind turbines and photo voltaic cells have entered the scene forcefully, and in our view, biomass should be reserved for higher value products," says Irini Angelidaki, continuing:

"I do not mean to say, that biomass should not be feedstock for energy production. For instance, we do produce biogas in the project with KMC. However, we do not think bioenergy should be the sole focus, but rather an element in a suite of products. Therefore, the name Bioconversions more accurately reflects what we do."

The project on valorization of potato starch effluents is funded by Innovation Fund Denmark as part of the InWAP program (Industrial Wastewater Valorization). The project will continue until summer 2022. Minmin Pan has completed his PhD degree and is currently employed in industry. Moreover, the group is going to continue activities for valorizing industrial wastewaters to high value products with a new EU project co-funded by Innovation Fund Denmark, the BlueBioChain project, with both KMC and DTU as participants.

🔺 Irini Angelidaki, Professor



A three-steps process for production of astaxanthin from a by-product from potato industry. 1. Potato starch by-product pretreated by anaerobic digestion, 2. The AD effluent is used for production of the microalgal biomass *Hamatococcus pluvialis*, 3. *H. pluvialis* is then induced for astaxanthin production. The AD effluent is used for production of the microalgal biomass *Hamatococcus pluvialis*, 3. *H. pluvialis* is then induced for astaxanthin production.

The BioConversions group BioCon

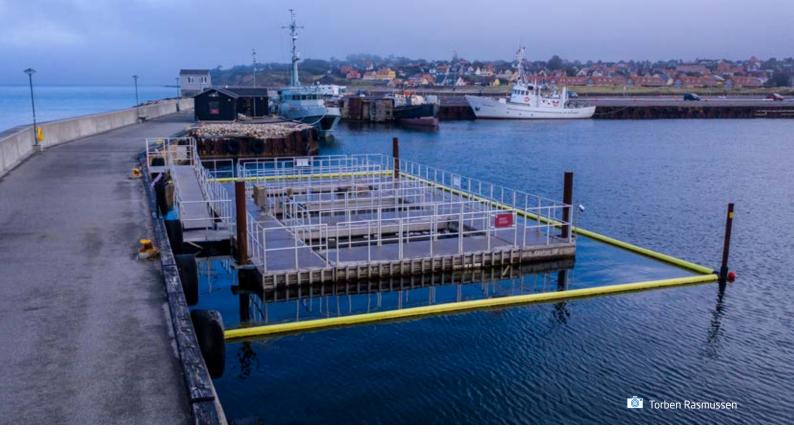
In the Biological Conversions group (Bio-Con), our goal is to develop and validate novel technologies exploiting microorganisms as tools to transform organic waste and wastewater into useful bioproducts, biofuels, and bioenergy.

Utilizing our expertise on 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 applied 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_2 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 CH₄) for grid injection. Demonstrating an efficient and high-rate CO₂ capture, utilization and storage technology can markedly combat global warming. In accordance with the European Green Deal to transform EU to climateneutral 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.



Give us fouling, please!

While shipowners hate seeing fouling on their vessels, coating researchers need aggressive biology to test innovations.

Calmly following the movements of the waves, a raft floats inside the Port of Hundested on the Northern coast of Zealand. The flat, hollow concrete construction is a new facility added to the experimental portfolio of CoaST (The Hempel Foundation Coatings Science and Technology Centre) at DTU Chemical Engineering. Here, the CoaST researchers can subject painted samples to real-life conditions.

"Lab experiments allow us to test a wide range of physical and chemical properties of a proposed coating, but seeing what happens when the coating is exposed to real-life conditions takes us to a new level of insight," says Claus E. Weinell. As Senior Executive Officer he is responsible for experimental facilities in CoaST.

The two main areas of tests in Hundested are anti-fouling and anti-corrosion.

Real sea water is the best test

Most anti-fouling coatings for ships contain active biocides which are released gradually over time to provide protection against fouling species for as long as possible. A core activity in CoaST is development of anti-fouling coating candidates with improved sustainability properties.

One area of research is coatings that do not contain biocides. It has transpired that it is possible to limit fouling through modification of the coating surface at the microlevel. Another area of research is coatings with more environmentally benign biocides, and a third area is coatings with controlled release of a smaller amount of biocide.

"Sustainability is a high priority in the shipping industry, but we need to ensure that improved sustainability does not come at the expense of inferior technical properties. The coating needs to remain functional for at least the time until the vessel would anyway be due for a scheduled overhaul. This will often mean for a period of up till five years," says Claus E. Weinell.

Obviously, the researchers cannot wait five years to see whether the coating is still functional. Instead, they take to so-called accelerated testing. In designated lab facilities, samples will be subjected to various



types of stress. This could be large fluctuations in temperature and/or humidity and/ or salinity.

"However, the best way to test anti-fouling is exposure to real sea water with a natural content of algae and microorganisms."

Simulating a ship in motion

One might think that the cool Danish waters would have a low biological activity and thus be less attractive for anti-fouling testing.

"We were happy to find that the natural biology here in Hundested is very active. The activity we see during the summer period is probably not any lower than it would be in, say, a subtropical climate and not so far from what I have experienced in tropical waters. Therefore, we can say that a coating which works here will typically work just as well in other parts of the world," assures Claus E. Weinell.

The raft in the Port of Hundested can host more than 1,000 coating samples. Further, a rotating device is now mounted on the raft, which makes it possible to simulate a ship in motion.

"While some industrial coating suppliers do have similar facilities, very few exist at public research centres," says Claus E. Weinell, adding that several materials and designs were considered for the raft:

"Besides the possibility of hosting many samples, the hollow-concrete solution is highly stable. Many different researchers visit and apply their projects for longer or shorter periods, and we wanted to make sure that they can do so under very safe conditions. Our specialist and mechanical engineer in the technical staff, Nezam Azizaddini, has done a very good job designing the raft."

Imaging gives early results

While the natural biology in the Port of Hundested is quite aggressive, it will still take some weeks or even months for large-scale fouling to occur. Based on



imaging techniques being developed by PhD researcher Morten L. Pedersen, early detection is possible if a coating is not effective. This enables earlier adjustment, thus saving precious time.

Still, why is it so difficult to recreate fouling in the lab?

"Nature is complex: The growth of one species is often interlinked with the growth of other species. Real-life fouling develops in steps, and if one link is missing in your lab experiment, you are not getting it right. Therefore, having the facility in Hundested is so valuable," concludes Claus E. Weinell, adding that the facility will never make lab experiments redundant:

"The lab is the place where you can have highly controlled conditions, which will always be very attractive, especially in the early phases of development. Only through the combination of lab and real-life experiments will we get the full picture."

Claus E. Weinell, Senior Executive Officer

Sustainability as a common denominator

The floating raft in the Port of Hundested will soon be joined by a static vertical installation at the outer pier. Here, the coating samples will be subjected to three different environments; one constantly under water, one constantly subjected to the atmosphere, and one where water and atmospheric influence interchanges with the tide and waves, the so-called splash zone.

Among the ongoing larger projects in Hundested is a project by Industrial PhD researcher Tenna Frydenberg on coatings containing smaller amounts of biocides than conventional coatings. PhD researchers Marcel Butschle, and Sara Golbarg look at coating surface modifications that inhibit fouling. And PhD researcher Shujie Lin investigates and develops methods and strategies for optimal hull cleaning.

"The project of Shujie Lin is highly relevant for shipowners, since despite efforts to prevent fouling, it will sometimes occur. And then, what will be the best treatment? Choosing the optimal scheme for cleaning will involve considerations over costs and sustainability and will also depend on the coating in question. For instance, surface-modified coatings are more susceptible to mechanical damage and should be rinsed more gently than conventional coatings," explains Claus E. Weinell.

While the projects may seem different, they are all part of the same overall pattern:

"Sustainability is a common denominator for all the mentioned projects. And many interlinkages exist. For instance, development of coatings by Tenna Frydenberg, Marcel Butschle and Sara Golbarg will have implications for the choice of rinsing method, as investigated in the project of Shujie Lin."

The Hempel Foundation Coatings Science and Technology Centre

CoaST

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 that must fulfil 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 must also provide, e.g., substrate protection such as resistance against corrosion or biofouling, provide longer escape times during a fire, or remove pollutant through catalytic activity.

Within the area of sustainable coatings science and engineering, CoaST aims 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
- Future 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 programmes 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.

Carbon capture by alkali absorption

A Danish-Dutch partnership investigates an entirely new approach to carbon capture. Lab results suggest the method may disrupt the industry.

Three industrial plants in Denmark, Greece, and Romania will become the sites for the first demonstrations of an entirely new carbon capture technology. While amine-based solvents have been the mainstream capture method for several decades, the new projects will use alkali absorption coupled to a novel electrodialysis cell.

"The main advantage of the method is low energy consumption. Since energy costs weigh heavily in amine-based capture, this could be a game changer. The results obtained in the lab are at a disruptive level. The question now is whether we can obtain the same in the demonstration projects," says Senior Project Manager Sebastian Nis Bay Villadsen, AT CERE (Applied Thermodynamics—Center for Energy Resources Engineering), DTU Chemical Engineering.

The three upcoming demonstrations will take place at Aalborg Portland's cement production site, at the Yerakine Mine in Greece, and at OMV Petrom's Petrobrazi refinery in Romania respectively. The demonstrations are part of a larger EU-funded project named ConsenCUS on carbon capture use and storage (CCUS).

Easy solvent regeneration the main advantage

The alkali absorption method is developed by Dutch technology centre Wetsus, also a ConsenCUS partner.

"Wetsus has demonstrated the potential of the method in their labs. However,

they need our expertise when it comes to upscaling. This is where we have decades of experience. Tests and experiments will run in parallel. Some in lab scale at the Wetsus facilities in the Netherlands, some at pilot scale here at DTU, and later at demonstration scale at the three industrial sites. We plan to have extensive knowledge sharing all the way. It is important that we coordinate the experiments so results can be compared," explains Associate Professor Philip L. Fosbøl, Principal Investigator of the project at DTU Chemical Engineering.

In the Wetsus method, carbon capture takes place in the strong base potassium hydroxide, abbreviated KOH from its name in German. Commonly known as caustic potash, KOH has a high reactivity towards acids. Still, the main advantage does not lie in the capture ability itself, according to Sebastian Nis Bay Villadsen:

"Once you have captured CO_2 , you need to extract the CO_2 from your solvent—not only to either use or store the CO_2 , but also, importantly, to regenerate your solvent. In amine-based capture this can only be achieved through a relatively large energy input. The real revelation by our Dutch colleagues is that the CO_2 can easily be extracted from KOH using electrodialysis."

Too early to call a winning technology

The group at DTU does not plan to abandon its activities in amine-based carbon capture:

"It would be premature to call a winning



technology. After all, the amine-based techniques have been optimized through several decades of fine engineering. But then again, when you have a technology which is cheaper, we know that things can suddenly happen very fast. Still, the most likely scenario seems to be that the two techniques and probably more will exist side by side," notes Philip L. Fosbøl, continuing:

"If we succeed in lowering the energy costs, and thereby lower the costs of operating the capture units, a new dynamic will come into play. We will see a shift from focus on cost of operation to cost of building the capture units. This will involve questions like which materials are needed, what do they cost at the time, and will it be possible to use smaller amounts of materials through optimization."

A further issue will be the price of electric power versus the price of heat, adds Sebastian Nis Bay Villadsen:

"Amine-based units are normally able to use excess heat from nearby facilities, while the Wetsus method will need electric power. Historically, electric power has been more costly than heat, but this may change due to positive developments in wind power, solar power, etc. These questions are all outside the scope of what we do in our group, but they may have a large impact when decisions are made on which technology to go for. In any case, we find it wise to engage in more than one capture technology."

Assembly work at DTU

In the project, a mobile unit will be built. The first demonstration is scheduled for Aalborg Portland's cement production site with likely inauguration by late 2023.

"Since a major part of the assembly work will take place here at DTU, it was natural to plan for the Danish site as the first place of demonstration," says Sebastian Nis Bay Villadsen.

Once in operation, the Aalborg demonstration facility is planned to run for five months. The demonstration cycle will include a preliminary test and a parametric screening study. The mobile unit will then be moved to Greece and later to Romania, also operating five months at each of these sites.

In Greece, the unit will be installed close to a rotary kiln at the Yerakini Mine in Chalkidiki. The mine is operated by Grecian Magnesite. Long-term test cycles will focus on solvent stability and accumulation of unwanted residues. The scope of the test cycles is to perform more than 1,000-hour tests.

In Romania, the unit will be installed at the OMV Petrom's Petrobrazi refinery. Longterm test cycles will focus on solvent stability and again, the aim is +1,000-hour tests. "Since the exhaust gases are quite different in cement production, in magnesite mining, and at a refinery, we will be able to test the technology under different, relevant conditions," notes Sebastian Nis Bay Villadsen.

- Sebastian N.B. Villadsen, Senior Project Manager
- Arrow Philip L. Fosbøl, Associate Professor

AT CERE manages DKK 34 million

The overall budget of ConsenCUS is the equivalent of DKK 100 million. Hereof approximately half is for the technical demonstration projects, and the DTU team will manage the DKK 34 million.

It should be noted that ConsenCUS is about more than technical demonstrations. The other half of the total budget is dedicated to other sides of CCUS, not least building industrial clusters and engaging with local communities around CCUS. Further subprojects will include conversion of captured CO_2 into formate and formic acid, and safe cyclic loading of CO_2 into salt formations and aquifers for storage.

ConsenCUS is just the most recent example of the carbon capture group at AT CERE being part of a successful European consortium within CCUS. Over the last two-three decades, the group has consistently taken part in all major EU programmes in the field.

Applied Thermodynamics-Centre for Energy Resources Engineering

AT CERE

The AT CERE Research Centre is focused in the areas of applied thermodynamics, transport properties and processes, materials science, fermentation technology, and mathematical modelling with applications in the energy sector incl. petroleum technology, CO₂ 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 covering 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 performing 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 carried out. Many of the applied problems are inspired by or based on input from CERE's industrial consortium.

Our history

In its various forms, AT CERE has a 30+ year 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 1980s 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 programme 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 also offered 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.

Highlights 2021

1 JANUARY NEW RESEARCH GROUP

On 1 January 2021, a new research group joined the Department. The new Bioconversions (acronym BioCon) is headed by Professor Irini Angelidaki. The group works with developing and validating new technologies based on the use of microorganisms as tools to transform organic waste and wastewater into useful bioproducts, biofuels, and bioenergy.

25 JANUARY FOURTH KT-IPE SEMINAR

The 4th KT-IPE seminar was held online. A total of 45 people participated in the plenary meeting. Before the meeting, six group meetings were held. Professor and Head of Department Kim Dam-Johansen and Professor and Director of IPE Suojiang Zhang summarized the progress of cooperation since the last seminar. The discussion in the group meetings were presented by the chairs in each group from KT (DTU Chemical Engineering) and IPE (Institute of Process Engineering). Former PhD students and postdocs connected to the DTU-IPE cooperation and now working at DTU and IPE shared their experiences in Denmark and in China.

FEBRUARY MOST CITED PAPER

The paper 'Screening of Catalysts for Hydrodeoxygenation of Phenol as a Model Compound for Bio-oil' in ACS Catalysis from 2013 was selected as being the most cited paper with authors from Denmark or Sweden since the birth of ACS Catalysis. Among the authors from the Department are Associate Professor Peter A. Jensen and Professor Anker D. Jensen.



FEBRUARY CO₂ CAPTURE ACTIVITIES

This year, many carbon capture projects have been launched at the Department. Back in February, a mobile carbon capture plant developed at DTU Chemical Engineering was connected to a functioning biogas plant at Mølleå wastewater treatment plant for the first time. This was the first stop for the demonstration plant. The aim was to demonstrate that it is possible to make carbon capture more profitable and upgrade biogas to valuable resources. On 24 June, a pilot carbon capture plant was launched at the waste-to-energy plant ARC in Copenhagen to test if energy-neutral CO₂ capture is possible by using the surplus heat from the process in the district heating network. The pilot plant can capture 850 tonnes CO₂ per day, and the goal is to capture 500,000 tonnes CO₂ per year by 2025. The plant has been established in collaboration with DTU Chemical Engineering, ACR, Pentair, Rambøll and EUDP (The Danish Energy Agency). Present at the launch were Associate Professor Philip Fosbøl, Danish Minister for Climate and Energy and Public Utilities Dan Jørgensen, and Copenhagen Mayor Lars Weiss.

8 MARCH NEW VISION IN PERSPECTIVE PAPER

Wastewater treatment plants provide sanitation and clean water. However, some may contribute to global climate change in form of N_2O emissions. In a perspective paper on NPJ Clean Water, Professor Gürkan Sin and Dr Resul AI (former postdoc at the Department) outline a vision for a multidisciplinary research field integrating gene sequence data into process modelling through deep learning/AI techniques to better model and operate these plants.



12 APRIL Horizon 2020 Project-Uplift plastics

Kick-off in the EU project targeting recycling of bio-based plastics and production of new Sustainable Plastics for the Food and Drink Packaging Industry. DPC is partner in the project with Associate Anders E. Daugaard.



22 APRIL John Woodley Receives Erc Advanced grant

Professor John Woodley received an Advanced Grant 2021 from the European Research Council (ERC) for his project 'Understanding the Effect of Non-natural Fluid Environments on Enzyme Stability'. The aim of the project is to improve our understanding of enzyme stability and broaden the field of potential applications for biocatalysis.

APRIL INTUMESCENT COATING REACH THE FRONT COVER OF I & EC RESEARCH JOURNAL

In relation to the publication: Dreyer, J.A.H.; C. Gunlach; C.E. Weinell; K. Dam-Johansen; S. Kiil (2021) Quantitative Characterization of Highly Porous Structures with Fluorescence Microscopy and Micro-Computed Tomography, Ind. Eng. Chem. Res. 60, 15. 5463-5470, https: //doi.org/10.1021/acs. iecr.0c06259, Postdoc Jochen Dreyer's illustration of intumescent coating was chosen as the front cover of I & EC journal's volume 60, issue 15.

12 MAY

INNOMISSION ROADMAP FOR GREEN FUELS IN TRANSPORT AND INDUSTRY

More than 100 companies, knowledge institutions, and cluster organizations have joined forces and developed a road map for how to phase out fossil fuels in the industries; heavy goods road transport, aviation, and the maritime shipping industry. The road map was submitted to Innovation Fund Denmark and was selected as the winning road map among several submitted roadmaps. The road will form the basis for a partnership application. The work was headed by Professor Anker D. Jensen.

Highlights 2021

15-17 JUNE KT CONSORTIUM ANNUAL MEETING

This year, the KT Consortium Annual Meeting 2021 took place online joined with the CERE Discussion Meeting 2021, following a similar format as previous years. The KT Consortium Annual Meeting had industrial participation in all the sessions, and more than half of the registered industrial participants (44 registered participants) attended plenary lectures. On the agenda were industrial talks from several large companies: AVEVA, NESTE Engineering, IBM together with TotalEnergies and Shell (invited by CERE) and a special session on biorefineries systems engineering (for RENSENG II project). At the meeting, the member companies expressed their view on the most important topics via a survey that showed the following: (1) PSE and Properties and Thermodynamics are the most important areas for their members; (2) the most important deliverables are the Annual Meeting, the member website, the publication list, and availability of just accepted manuscripts together with (3) availability and development of ICAS software and its tools.



21 JUNE TWO NEW ACADEMY MEMBERS

Professor Georgios M. Kontogeorgis and Professor Krist V. Gernaey have both been admitted members of ATV—the Danish Academy of Technical Sciences along with 38 other technology leaders and top researchers.



21 JUNE ELASTYRENPRISEN TO ANDERS

E. DAUGAARD Associate Professor Anders E. Daugaard received the Danish polymer award ATV Elastyrenprisen. He received the award for his "internationally prominent research, great commitment to knowledge-based dissemination and teaching, as well as exemplary research in bio-based plastic materials and recycling of plastics. His results are impressive, and he has managed to convey a technical understanding of plastic materials to a wider audience".

14-16 JUNE

CERE DISCUSSION MEETING

The 2021 CERE Discussion Meeting was held online. The programme consisted of both plenary and parallel sessions, with a total of 50 oral presentations—a testimony to the size and the health of the centre. Also, four invited industrial talks was on the programme: Daniel Künisch Eriksen from Shell; Nevin Gerek Ince from Aveva; Niels Lindeloff from TotalEnergies and Susanna Kuitunen from Neste. The last two in collaboration with KT Consortium. The number of online participants was high with 140 registrations.

25 JUNE ONLINE GREEN CHALLENGE

Three groups of SDC students joined online the Green Challenge at DTU, and presented projects related to CO₂ capture and green production of chemicals.



22 JULY GOODBYE TO A GREAT CHEMICAL ENGINEER

In 2021, we lost a great and inspiring chemical engineer, and a good friend. Professor Emeritus John Villadsen passed away on 22 July 2021, marking the end of a long and distinguished career at DTU. Since officially retiring, John Villadsen remained a fixture at the Department, making significant contributions to the academic and social life of the Department as a 'Senior Professor' for 15 years. Right up until the end, he remained a great source of inspiration to all of us.

2 AUGUST

ANOTHER SIGNIFICANT DONATION TO COATINGS RESEARCH

The Hempel Foundation donated DKK 30 million to CoaST to support DTU Chemical Engineering's continuous research in coatings and the further development of The Hempel Foundation Coatings Science and Technology Centre, CoaST.

9-13 AUGUST SUMMER SCHOOL ON UNCERTAINTY & SENSITIVITY

Professor Gürkan Sin held the 12th edition of the Summer School on Uncertainty and Sensitivity Analysis of Engineering Models from 9-13 August 2021 at DTU Lyngby Campus. 31 participants (50 per cent outside of DTU, the majority from abroad) with multi-disciplinary and multi-engineering background followed this intensive one-week training event.

15 AUGUST

US NAVY RESEARCH FUNDING FOR ANTIFOULING COATINGS

Professor Søren Kiil received a two-year research grant from the US Navy to a project on 'Transparent biocide-based antifouling coatings'.



20 AUGUST RESEARCH DAY 2021

Once again, the entire Department gathered for the annual Research Day—this time in a hybrid form. External speaker Michael Paludan-Müller Nylykke from Ørsted gave a talk on 'P2X paradigm—Coupling renewable energy with chemicals/fuels'. The winners of this year's PhD video workshop competition were PhD students Aixiao Fu and Zhiwei Wu, demonstrating great science communication skills with the use of their smartphones.



Highlights **2021**



27 AUGUST COAST MARITIME TEST CENTRE EXHIBITION

The opening of the small exhibition on coatings at the CoaST Maritime Test Centre at the Port of Hundested marked the completion of the CoaST Maritime Test Centre—a state-ofthe-art test centre offering in-situ exposure of samples to a marine environment. Samples can be exposed by full immersion in the splash/tidal zone as well as in the atmospheric marine environment. Further, the exposure can be static or dynamic mimicking vessel speed up to 35 Knobs.

6 SEPTEMBER NEW WASTE TECHNOLOGY TO REDUCE CO2 EMISSIONS

Earlier this year, the Innovation Fund Denmark granted DKK 18.6 million to develop technology that reduces CO₂ emissions from cement factories and delivers fuel with a low CO₂ footprint. Initiated by FLSmidth and DTU, the project is headed by DTU Chemical Engineering and also consists of DTU Management, FLSmidth, Dampskibsselskabet Norden, MAN Energy Solutions SE, Topsøe, Geminor, and Finnsementti Oy.

4-6 OCTOBER SECOND AIM-BIO SYMPOSIUM

The second AIM-Bio symposium with 70 participants from DTU, NC State University, and the biotech industry was held in hybrid format at DTU.



15 OCTOBER PROSYS ANNUAL RESEARCH SEMINAR

The PROSYS Research Seminar was held as a hybrid event for about 175 participants, including about 100 from our external partners. Ralf Takors (University of Stuttgart), Anette Birck (Helix Lab Kalundborg), and Maria Rumbau (Aquaporin) attended as external speakers.

15 OCTOBER FUNDING FOR NEW TYPE OF COATING

Professor Anne Ladegaard Skov received funding from the Independent Research Fund Denmark to the project 'Liquid coatings with no use of solvents'. The goal is to replace Volatile Organic Compounds (VOC) with a new type of eco-friendly coating.



30 OCTOBER-6 NOVEMBER FBM OUTREACH TRIP

As a part of the FBM PhD programme, eight PhD students from DTU Chemical Engineering, DTU Bioengineering, and DTU Biosustain went on an outreach mission to visit companies and universities in the Netherlands, Belgium, and Germany to establish new connections for future collaborations and to get insights into industrial biotechnology in other countries.



11 NOVEMBER CHEC ANNUAL DAY

The CHEC Annual Day was held as a hybrid meeting. In total, 80 people attended physically, hereof 30 external guests. Around 23 external guests attended online. The meeting also featured six talks on future processes from external collaborators: Haldor Topsøe; Mærsk McKinney-Møller Center for Zero Carbon Shipping; MAN Energy Solutions; Rockwool; FLSmidth and Stiesdal Fuel Technologies.

30 NOVEMBER DIGITAL TECH SUMMIT 2021

At the Digital Tech Summit 2021 in Copenhagen, Professor Krist V. Gernaey participated and coordinated the session 'Pharmaceutical production 'Digital Twin': Digitalisation of Biomanufacturing Operations'.

Cooperating companies

3

3V TECH EQUIPMENT & PROCESS SYSTEMS SPA

Α

Alfa Laval Applied Chemicals and Materials Division, NIST Aquagreen Aquaporin ARC ARKEMA FRANCE Arla Foods Ingredients Group AVEVA AWAPATENT

В

Babcock & Wilcox Vølund BASF Bayer Biomar Biopro Bioscavenge Biosyntia Blue Chemney BP BTG Bioliquids Burkert

C

Calsep Carlsberg Research Laboratory Centro Tecnológico Componentes Chempilots Chevron Chr. Hansen Chreto Ckj Steel C-LEcta Coloplast Contura Covestro Deutschland CP Kelco

D

Dall Energi Dampskibsselskabet Norden Dansk Gasteknisk Center Dan-Unity DHI DSM DTI DuPont Nutrition and Biosciences Denmark

Ε

Electrochaea.dk Elkem Elysium Robotics EnCoat Engineering Consulting Corporation EnviDan Equinor

F

Finnesementti Firmenich FlowLoop FLSmidth Fluidan Fluor Corporation Foodture Freesense Fujifilm Diosynth Biotechnologies

G

GEA Process Engineering Gelest Geminor GLYCOM Denmark GR3N SAGL Grundfos

Η

Haldor Topsøe HCS Hempel (H&M) HENNES & MAURITZ GBC Holm Christensen Biosystemer Hundested Havn

IFEN IFP Energies nouvelles Innosyn Insatech

] Jar

Janssen -pharmaceutical company of Johnson & Johnson Jiangsu Industrial Technology Research Institute

Κ

Kalundborg Forsyning Karup Kartoffelmelsfabrik (KMC) KBC KMT Cables

L

Landbrug & Fødevarer LEAP Technology LEGO Lemvig Biogas Leo Pharma Linde Liqtech Lundbeck Lundbeck Lundsby Biogas

Μ

Madsen Bioenergi MAN Energy Solutions Mash Energy Microsoft Mitsubishi Multiflex folien Mölnlycke

Ν

NEO GROUP Neste Jacobs Nordic Sugar Nouryon Nova Pangeae Novartis Novo Nordisk Novozymes

Ρ

ParticleTech Pharmacosmos PK Chemicals Polyloop Pond Process Design PROCESSI INNOVATIVI Processium

Q Q-Interline

R Resino

Rockwool

S

Saltkraft Scienciox Shell Siemens-Gamesa Sinopec Solchroma Stiesdal Fuel Technologies SYNESIS Syngenta

Т

Teknologisk Institut TOTAL Toyada Gosei

U

Ucomposites Umicore Denmark Unibio Group Unilever Union Engineering US Navy, Office of Naval Research

V Valmet Veolia

W

Wacker Chemie Waste Plastic upcycling Wintershall WPU

X Xellia Pharmaceuticals



A new KTStudents board

The student organization KTStudents works to improve the study environment for students through social and professional activities. Despite a challenging year with partial lockdown, a new board and an increase in members have added new spark to the student organization.

2021 was in many ways a turbulent and ambivalent year for the student organization.

"We were under partial lockdown during the spring semester. This meant that we were only able to arrange online events, which had limited attendance. We also had a large turnover of board members, as most students either graduated or went on exchange," says Simon Knudsen, Chairman of KTStudents.

But every cloud has a silver lining. After the lockdown, KTStudents saw a large boom in both member applications and attendants to events. During the general assembly in the fall, an impressive 80 students signed up.

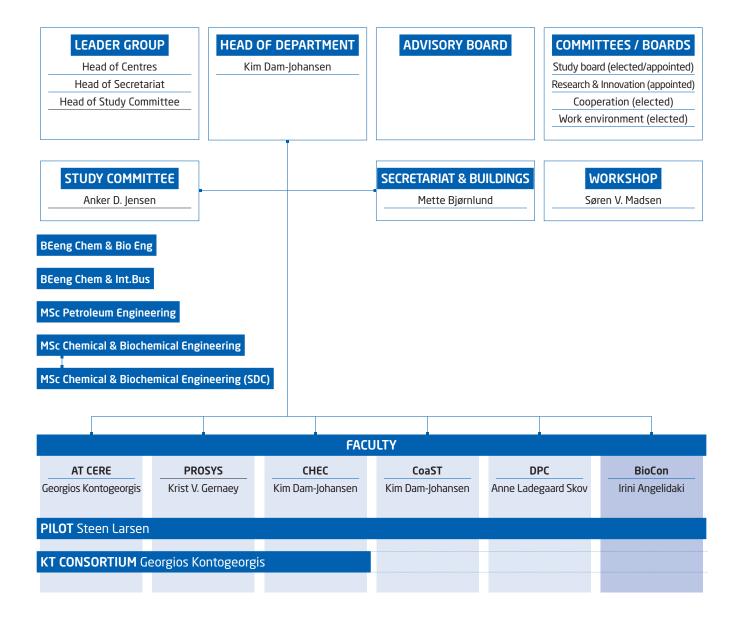
"I think 2022 will be a fun year to be part of KTStudents. We have planned two company visits—one at Hempel and another at Haldor Topsøe. We have also successfully applied for an ISN grant of DKK 50,000 dedicated to the revival of the good student life, which we plan to use to encourage vulnerable and isolated students to meet new friends and engage in the community, increase social cohesion, and arrange academic and professional events on a larger scale than before. KTStudents has not just survived the corona pandemic, it has been renewed in many ways," Simon concludes.

Simon Knudsen, Chairman of KTStudents



KTStudents board. From left to right: Gauri Undegaonkar, Melissa Rugholm Jensen, Guilheme Frizado, Simon Knudsen, Yashomangalam Bhutada, Rikke Vilsøe, Oskar Bek Jørgensen, Cristina Hotea

Organization



The Faculty **2021**

SCIENTIFIC



Anders E. Daugaard Associate Professor



Anne Ladegaard Skov Professor











Hao Wu Associate Professor

Hariklia N. Gavala Associate Professor



Helena Junicke Assistant Professor



Ioannis V. Skiadas Associate Professor



Irini Angelidaki Professor



Jakob K. Huusom Associate Professor





Jakob M. Christensen Associate Professor

Jens Abildskov Associate Professor



John Woodley Professor



Kim Dam-Johansen Professor, Head of Department









Martin Andersson Associate Professor



Xiaodong Liang Associate Professor



Peter Glarborg Professor



Associate Professor

ADMINISTRATIVE





Seyed S. Mansouri Associate Professor



Søren Kiil Professor

Ulrich Krühne Associate Professor





EMERITUS

Mette Bjørnlund Head of Secretariat



Gunnar E. Jonsson Associate Professor Emeritus



Khosrow Bagherpour Senior Consultant PILOT PLANT

John Villadsen Professor Emeritus Kaj Thomsen Emeritus

Lars G. Kiørboe Emeritus



Ole Hassager Professor Emeritus



Sten B. Jørgensen Professor Emeritus



45











Teaching

The Department participates in two 3½-year Bachelor of Engineering (BEng) programmes, one in Chemical and Biochemical Engineering, and one in Chemical Engineering & International Business, a three-year Bachelor of Science (BSc) programme in Chemistry and Technology, three two-year Master of Science (MSc) programmes in Applied Chemistry, Chemical and Biochemical Engineering, which includes an Honours programme, and Petroleum Engineering, 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 modelling, process and product design.

Courses

1 SEPTEMBER 2020-31 AUGUST 2021

PHD COURSES

28904	Polymer physics
28905	Advanced topics in process systems engineering
28908	Rheology of complex fluids (heavy)
28909	Thermodynamic models, fundamentals, and computational
	aspects
28917	Statistical thermodynamics 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 engineering
28932	Process engineering laboratory

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 2020-2021, 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 (84)
28012	Chemical and biochemical process engineering (79) (B)
28016	Mathematical models for chemical and biochemical systems
	(78) (B)
28020	Introduction to chemical and biochemical engineering (72)
28022	Unit operations of chemical engineering and biotechnology
	(99) (B)
28121	Chemical unit operations laboratory (11)
28125	Chemical unit operations laboratory (5)
28140	Introduction to chemical reaction engineering (39)
28150	Introduction to process control (26)
28157	Process and product design (51) (B)
28213	Polymer technology (28)
28233	Recovery and purification of biological products (122)
28242	Chemical kinetics and catalysis (54)
28244	Combustion and high temperature process (49)
28310	Chemical and biochemical product design (51)
28315	Colloid and surface chemistry (67)
28316	Laboratory course in colloid and surface chemistry (13)
28322	Chemical engineering thermodynamics (75) (B)
28342	Chemical reaction engineering (50) (B)
28344	Biotechnology and process design (22) (B)
28352	Chemical process control (54) (B)
28420	Separation processes (45)
28455	Process adaptation in fermentation-based
	biomanufacturing (57)
28480	Biobusiness and process innovation (152)
28515	Enhanced oil recovery (13)
28530	Transport processes (52)
28831	Computational fluid dynamics in chemical engineering (10)
28845	Chemical reaction engineering laboratory (24)
28852	Risk assessment in chemical industry (42)
28864	Introduction to Matlab programming (26)
28870	Energy and sustainability (107)
28872	Biorefinery (44)

COURSES GIVEN IN COOPERATION WITH OTHER DEPARTMENTS:

23522	Rheology of food and biological materials (24)	

- **26010** Introductory project in chemistry (71)
- **41686** Materials science (19) **(B)**

SPRING SEMESTER

28012	Chemical and biochemical process engineering (50) (B)
28016	Mathematical models for chemical and biochemical systems
	(34) (B)
28020	Introduction to chemical and biochemical engineering (72)
28022	Unit operations of chemical engineering and biotechnology
	(33) (B)
28025	Bio process technology (25)
28121	Chemical unit operations laboratory (26)
28157	Process design (29) (B)
28160	Mathematical models for chemical systems (44)
28212	Polymer chemistry (47)
28214	Polymer synthesis and characterization (12)
28216	Organics coatings science and technology (11)
28221	Chemical engineering thermodynamics (11)
28231	Laboratory in chemical and biochemical engineering (16)
28271	Thermal gasification and sustainability (14)
28322	Chemical engineering thermodynamics (36) (B)
28342	Chemical reaction engineering (70) (B)
28344	Biotechnology and process design (45) (B)
28345	Chemical reaction engineering (71)
28350	Process design: Principles and methods (62)
28352	Chemical process control (32) (B)
28361	Chemical engineering model analysis (55)
28415	Oil and gas production (9)
28423	Phase equilibria for separation processes (25)
28434	Membrane technology (60)
28443	Industrial reaction engineering (39)
28451	Optimizing plantwide control (23)
28535	Rheology of complex fluids (light) (3)
28850	Quality by Design (QBD): Integration of product and process
	development (79)
28855	Good manufactoring practice (116)
28864	Introduction to Matlab programming (53)
28871	Production of biofuels (34)
28885	Technology and economy of oil and gas production (13) (B)

COURSES GIVEN IN COOPERATION WITH OTHER DEPARTMENTS:

- 12701 Introduction to living systems (60)26317 Instrumental chemical analysis (45)
- **27455** Microbial adaptation to industrial processes (61)
- 41686 Materials science (82) (B)
- 41687 Exercises in materials science (39)

BACHELOR OF ENGINEERING DEGREES

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

Amidation of MeSA under high temperature and pressure conditions Digital twin of batch distillation Hydrogen storage for sustainable future under Power to X theme Sustainability in off-shore oil and gas production (3 students) CIP cleaning of hollow fiber membranes for forward osmosis applications (2 students) Data-driven analysis of biprocesses using non-invasive measurements Demonstration of advanced CO₂ capture in pilot scale Design and construction of a pilot scale test plant for fluid dynamic investigations Recovery of HMF from aqueous reactive solutions A hybrid, computer-aided approach for maintaining high productivity of analytical chromatograph An overlooked global warming challenge: The issue of waste anesthetics (3 students) Installation of an automatic vapor barrier in the distribution line to a fermenter as a measure to save vapor and energy Iron as energy carrier (2 students) Crosslinked microspheres prepared from biopolymers Equilibrium constants for biocatalytic reactions (2 students) Modeling of biochemical reaction equilibria Measurements of CO₂ capture kinetics, and the impact of additives (2 students) Deviation creation criteria Optimization of the biological removal of phosphorus at HCR Syd Wastewater Treatment Plant Optimization of the catalytic working area focusing on safety procedures and the drying process of the diesel particulate filters Optimization of low-CO₂ geopolymer cements Flow reactor oxidation of CO/NH₃ mixtures High pressure oxidation of NH₃ Oxidation of NH₃/fuel mixtures at high pressure Pilot optimization and solvent analysis from CO₂ capture (2 students) Process design and analysis of a method for destructing waste anaesthetics PVA as an additional layer inside hollow fiber forward osmosis membranes for improved rejection and anti-fouling behaviour. Techno-economic analysis of mitigating waste anesthetics towards commercializing a new sustainable technology Thermogravimetric study of iron as energy carrier Development and evaluation of catalysts for methanol-synthesis from carbon monoxide Development and characterization of an integrated system to destruct waste anesthetics Investigation of colorimetric sensors applications Study of the foaming effect of process fluids on relative cleanability Investigation of water scavenging methods for moisture curing sealants BACHELOR OF SCIENCE DEGREES 24 students finished their research programme for the BSc degree. The project titles are listed below:

Sulphur deactivation of close coupled SCR catalysts for diesel vehicles (2 students) Mechanical properties and modelling of skin adhesives Optimized biochar production on a two-stage biomass gasifier Inorganic intumescent coatings Development of a heterogeneous catalyst for synthesis of acetonitrile based on ammonia and methanol Application of nano-biochar in soils for nitrous oxide (N₂O) emission mitigation (2 students) Periodic stripping (2 students) Properties of CO₂ capture solvent Experimental study of hydrodynamics in a dual circulating fluidized bed system Catalytic pyrolysis of plastics (2 students) Equilibrium constants for transamination reactions Modelling of a pilot scale chromatographic process Modelling of soil carbon changes following application of straw biochar in Danish soils Oxidation of ammonia under Rockwool cyclone conditions Stabilization of pyrolysis bio-oil model compounds by hydrogenation Ammonia synthesis by plasma catalysis Intumescent coating testing using a radiant heater Investigation of external acidity of H-ZSM-5 zeolites **(2 students)** Validation of a simulation model for cyclic separations

MASTER OF SCIENCE DEGREES

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

3D Inject-printing photo-crosslinkable resins for optical components 3D optical scanning technology as an in-situ process control Trigger point activation of simulation-based industrial capacity problems Soft-sensors application and big-data generation in mammalian cell cultures Application of flow cytometry for the analysis and optimization of recombinant scFv13R4 production in Pichia Pastoris Advanced image analysis for the automatic identification of fungi morphological features Designing a process for producing FAME from chemical biodiesel soap-stock Design of periodic operation of reactive separations Design of silane-epoxy resin systems for conditions of high pressure and high temperature (2 students) Design and operation of an intensified high-purity separation Effect of heating rate on intumescent coating performance Experimental and model-based analysis of denitrifying phosphorus accumulating organisms (dPAOs) in a full-scale Membrane Aerated Biofilm reactor (MABR) Experimental study on the activation of biomass char using residues from sodium carbonate industrial production Energy integration through retrofitting of heat exchanger network at Equinor Kalundborg Oil Refinery Corrosion resistance of epoxy resins modified by silanes at high pressure and high temperature conditions Fermentation of syngas to methane in trickle bed bioreactors: Optimization of pilot scale operation Flow visualization in a waste to energy power plant Biopolymer blends prepared for improved processability of bioplastics Preparation of conductive PVA hydrogels on ceramic membranes In situ bio-succinic acid separation with electrolytic cell (2 students) Intelligent design of phase transfer catalysts using deep learning Calibration methods for chromatographic models (2 students) Cascade Enzyme immobilization on polyelectrolyte multilayer membranes Kinetics and transport processes in catalytic adiabatic post conversion in dry methane reforming Coupling water absorption and rheology of hydrated pressure sensitive adhesives Crosslinking of degradable microspheres into monolithic structures Quantification of immobilized vesicles on polymer surfaces Quantification of mechanical properties of two-component epoxy coatings during curing Mathematical modelling-Predictive maintenance and statistical process control Mechanical properties and modelling of skin adhesives Model based optimization of spray drying capacity for oral API Model for sulphur release from raw meal in cement production Modelling of a GFP producing bioreactor Modelling chromatography using a hybrid machine learning approach Modelling and optimization of a sustainable integrated biorefinery for the production of biofuel and bioplastics from organic waste Experimental verification of methane replacement in gas hydrates Methane production and CO₂ storage in a porous medium with promoter Numerical investigation of an industrial large-scale fed-batch cultivation Numerical investigation of the mixing conditions for oxygen in an industrial bioreactor Numerical investigation of industrial process conditions in bacterial cultivations and during separation Novel enzymatic approaches in liquefying corn/rice adjunct

Optimal drum filtration strategy in enzyme recovery (2 students) Optimization of anion exchange chromatography step with HTP screening for antibody purification Lab-scale optimization of succinic acid production and biogas upgrading: Focusing on Actinobacillus succinogenes 130Z strain improvement Optimizing adhesion of turbine blade protection system using plasma-assisted pre-treatment methods Phospholipases in the pretreatment of crude oil for biodiesel Production and characterization of biooil Pyrolysis and oxidation kinetics of bio-based binders used in stone wool products Synthesis and characterization of conjugated polymer-2D material composites for energy storage applications Set up of a testing protocol for topical and transdermal delivery of cannabinoids from silicone-glycerol adhesives Glucose oxidase stability studies Investigating how different practices of manure management affect methane emissions and biogas potential Investigation of the control and performance of wash & sterilization equipment in a biopharmaceutical company Fractionation of pyromix using membrane technology Quantification of CO₂ and H₂S gas emissions from Krafla geothermal power plant in Iceland Downscaling enzyme production Preparation of linear condensation polymers mimicking polyurethanes Recovery of ammonia from aqueous ammonia-soaked biomass Continuous catalytic hydrogenation of active pharmaceutical ingredients in a trickle bed reactor (2 students) Pilot scale enzymatic esterification of free fatty acids in crude biodiesel using a continuous bubble reactor system Process model development for a novel hemophilia drug substance using a hybrid machine-learning assisted modelling framework Production of aromatic amino acids and derivatives in E.coli 2D simulation of granular flow in a rotary kiln reactor Addressing plasmid stability and membrane space for biochemical production in E.coli Bioenergy potential analysis for houses and compounds of the United Nations in Africa Application of Graph Neural Networks for chemical property prediction Processing of seaweed for biological production of bulk chemicals Investigation of an ultrafiltration process with CFD modelling and microfluidic experiments Evaluation of microfiltration for hygiene improvements of liquid goods in downstream processing Multistage CH₄-CO₂ swapping in porous medium Characterization and significance of threads in bifidobacteria fermentation Quantitative physiology of the methanotrophic bacteria Methylococcus capsulatus (Bath) in a U-loop bioreactor Mechanical properties of crosslinked silicone-glycerol emulsions Off-gas test of raw meal for cement production Ammonia oxidation in a flow reactor The applicability of the theory of sampling in in-line and off-line particle size distribution measurements Silicone based drug delivery devices P2X sulphur removal technology simulation and pilot for biogas upgrading Understanding pigment dispersion for coatings (2 students) SDC MASTER DEGREES

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

Glucose oxidase stability studies Control oriented modelling of instant coffee - Freezing temperature predictions Nickle Tripyrrins as an electrocatalyst for H₂ evolution dependence on acid strength Experimental and numerical modelling studies of the mechanisms of ammonia oxidation and NOx formation in a fixed-bed reactor Stripping chlorine and sulfur from cement meal Design of coating layer for enzyme immobilization based on mussel-inspired phenol-amine chemistry Green process for catalytic carbonylation of 1,5-pentanediamine to pentamethylene dicarbamate over TiO₂ catalyst Role of carbon-oxygen complexes in NOX reduction by coal char Removal of trace amount impurities in glycolytic monomer of polyethylene terephthalate by recrystallization Fast catalytic pyrolysis of corn straw for deoxygenation and dechlorination of bio-oil

wastewater

Controllable polymerization of NCA catalyzed by chiral phosphoric acid

Multiscale reactive simulation of a novel catalytic cracking reactor for maximizing iso-paraffins

Stable nucleation of single nanobubble during electroreduction reaction in ionic liquids (2 students)

Nitrogen removal characteristic and genome-wide sequence analysis of efficient anaerobic denitrifying bacteria isolated from *Myriophyllum aquaticum* constructed wetlands

lonic liquids assisted morphology control of Nb2O5 and their catalytic performance for adiponitrile production

Measurement of suspended particles in aqueous [Bmim]BF4 solution using an online electrical sensing zone method

Fabrication and characterization of nanostructured transition metal phosphide electrocatalysts for seawater splitting

WoS publications

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