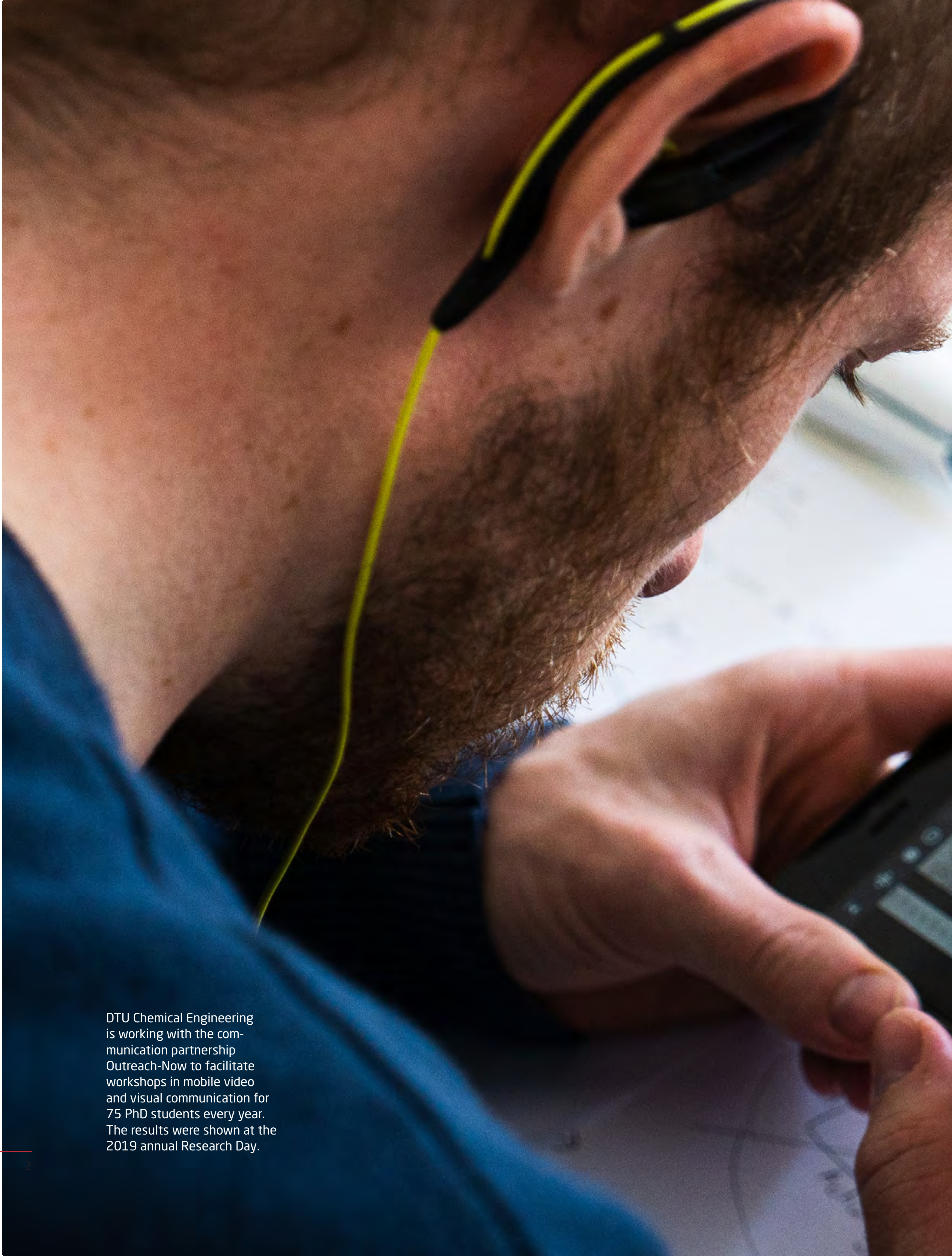
DTU

DTU Chemical Engineering
Department of Chemical and Biochemical Engineering

Annual report 2019



DTU Chemical Engineering is working with the communication partnership Outreach-Now to facilitate workshops in mobile video and visual communication for 75 PhD students every year. The results were shown at the 2019 annual Research Day.

Contents

Technological solutions for a sustainable future

Sustainability continues to be the main focus of an increasing number of stakeholders in our society. This have been a great focus at the Department of Chemical and Biochemical Engineering for a number of years as well. We strive to build fundamental knowledge to assist the industry in developing cutting-edge technological solutions, to the benefit of companies as well as society at large.

This year's annual report mirrors this striving. Going through its pages, you will see many concrete examples of technological solutions that are vital if we want to reach the political goal of reaching a 70 per cent reduction of CO_2 emissions by 2030 in Denmark, and if we want to support the UN SDGs in general.

We are researching carbon capture, storage, and utilization, as it is not sufficient just to reduce emissions—we also need to actively capture CO_2 and put it to new use. A similar mindset is applied in the Synferon project, where we are converting biomass into 'syngas', turning it into a resource rather than waste. And in another research case, we see how a start-up company can turn normally environmentally problematic sludge from waste water treatment into a resource.

But sustainability is many things, and we need to be smart in the way we approach the solutions. As you can also read in one of our articles, it can be argued that if we are able to recycle a fossil polymer many times, it might in fact be more sustainable than bio-based polymers. And as our work

in the collaboration between academia and industry shows, new software solutions can help companies to improve the sustainability of their products by predicting their biodegradability.

During the year, the relatively recent established Coating Science and Technology Centre, CoaST, has grown significantly, starting projects to facilitate the development of new sustainable coatings solutions under the headline ‘Coatings for a better future’.

These are all activities you can read more about in this annual report.

In many ways, 2019 was a year of transformation for our Department. Not only are we transforming sustainable technologies—we have also planned to move into brand-new surroundings in our new state-of-the-art research and education Building 228A. This is an important part of our growth as B228A offers new possibilities for both research and education.

Speaking of education, this year has seen the launching of the FBM initiative, a collaboration between different departments at DTU. It focuses on fermentation-based biomanufacturing and offers a unique and internationally leading education and research environment. This is important, as chemical engineering students today need a variety of different skills to work across many fields of research and innovation.

Also related to teaching, we have further developed our education in the framework of the Sino-Danish Center for education and research, SDC—and we have developed courses in Coatings Science and Technology to be taught in both China and Denmark.

New sustainable and innovative solutions are not a solo effort- it is a task that must be solved across, teams, centres, departments, universities, and industry. We have created a research and educational environment at DTU where this is more possible than ever before. And the transformation is far from over.

We are looking forward to significant growth in our cooperation with industrial and academic partners to the benefit of finding and implementing the best and most sustainable solutions.

Kim Dam-Johansen
Professor, Head of Department

Kim Dam-Johansen
Professor,
Head of Department

Key numbers **2019**

208
SCIENTIFIC ARTICLES IN WOS-INDEXED JOURNALS

9
REPORTS AND BOOKS

33
PHD DEFENCES

327
STUDENTS*

24
COMPLETED BSC PROJECTS

41
COMPLETED BENG PROJECTS

74
COMPLETED MSC PROJECTS

31
SINO-DANISH STUDENTS

5

SPIN OUTS

8

NOTIFICATIONS OF INVENTION

47

TECHNICAL/ADMINISTRATIVE EMPLOYEES**

96

PHD STUDENTS INCLUDING 11 INDUSTRIAL PHDS**

32

VISITING GUEST RESEARCHERS FROM 16 DIFFERENT COUNTRIES

87

SCIENTIFIC EMPLOYEES**

230

EMPLOYEES IN TOTAL**

34

FACULTY MEMBERS

* BASED ON STÅ. ONE STÅ IS THE EQUIVALENT OF ONE STUDENT STUDYING FULL TIME IN A YEAR
** BASED ON FULL TIME EQUIVALENT (FTE)

A greener version of carbon capture

Lowering CO_2 emissions is no longer considered enough to preserve the Earth's climate. We also need to actively capture CO_2.

According to the IPCC (the International Panel on Climate Change), the world will need not only to get to zero carbon net emissions by 2050. If we are to preserve the present climate, we even need to achieve negative emissions.

"Saying negative emissions is another way of saying Carbon Capture and Storage (CCS)," says Associate Professor Philip L. Fosbøl, AT CERE, DTU Chemical Engineering.

"Even with a full transition to renewable energy, we will still need to produce goods which are bound to emission of CO_2. We cannot just stop using steel, cement, medicine, paper, and similar types of welfare goods which all rely on processes that emit a noticeable amount of CO_2. Therefore, we will not be able to do without carbon capture. In other words, we should invest in CCS just like we invest in renewable energy technologies," he continues.

DTU Chemical Engineering has pursued CCS consistently, regardless of changes in political interest over the years. Not least has participation in all major EU programmes over the last two decades allowed a high level of activity in the field.

"Carbonic anhydrase is one of the fastest enzymes known. This is highly attractive in relation to carbon capture, as we typically need to capture CO_2 from huge amounts of flue gas."

Enzyme from blood to the rescue
A major challenge in CCS is reducing the energy consumption required for capturing the CO_2. A high energy consumption will both be damaging to the sustainability of the method and to the economic feasibility. Therefore, it is good news that the researchers at DTU Chemical Engineering have found a method which improves current state-of-the-art capture methods when it comes to energy efficiency.

The new method is based on addition of the enzyme CA (carbonic anhydrase). CA is found in human blood. In our body, the main function of CA is to enhance the mass transfer of CO_2 in our lungs by catalysing the reversible hydration of CO_2.

"CA is one of the fastest enzymes known. This is highly attractive in relation to carbon capture, as we typically need to capture CO_2 from huge amounts of flue gas. We have shown that CA is able to speed up CO_2 capture in an industrial context. While the enzyme isn't a CO_2 solvent in itself, it increases the capture capacity of the best commercially available solvents," explains Associate Professor Nicolas von Solms, also working in AT CERE.

The industrial state-of-the-art solvents for CO_2 capture are amines such as MDEA (methyl-diethanolamine).

"MDEA is a very efficient and specific solvent for CO_2 capture, but it is rather slow. You can compensate for this by increasing the size of your capture plant, but that would add to both building costs and energy consumption. The latter is problematic both in terms of operating costs and sustainability. By speeding up the capture process, we can operate a smaller facility."

A green additive
In terms of economic feasibility, the new method is currently not superior, because the cost of the CA needs to be factored in. Even though the enzyme is not consumed directly in the process—enzymes function like catalysts in an industrial plant, they facilitate the reactions between other compounds – some new CA needs to be added to keep the process going. The price of the enzyme will go down if and when more capture facilities adapt the method, allowing CA to be produced with economy of scale. Still, for some time the cost of the enzyme will imply that the new, more efficient process will have overall costs that roughly equal those of current CO_2 capture by amines without enzymes added.

"So initially, the advantage will not be economical, but by operating smaller and more energy-efficient plants, carbon capture becomes more sustainable. On top of that we're using a green additive, since enzymes are manufactured at biotechnological plants under mild conditions," Nicolas von Solms points out.

Carbon Capture at DTU Chemical Engineering

Some 8-9 researchers and a similar number of students are doing projects on carbon capture at DTU Chemical Engineering. The efforts are anchored in AT CERE (Applied Thermodynamics, Center for Energy Resources Engineering).

Fundamental research projects on the subject include the use of ionic liquids (ILs) as solvents for carbon capture, and swapping CO_2 for methane in gas hydrates, respectively. Both of these projects are coordinated by Associate Professor Nicolas von Solms.

Further, carbon capture plays a role in three ongoing projects with biogas as the common denominator. In the first project, MeGa-StorRE (Methane Gas Storage for Renewable Energy), methane is produced by removing CO_2 from the biogas. In the second project, Bio Re-fuel, CO_2 is also removed from the biogas, but instead of methane, the end-product will be methanol. The third project, BioCO2, focuses on utilizing the captured CO_2 as a valuable industrial feedstock. All three projects are coordinated by Associate Professor Philip L. Fosbøl. The MeGa-StoRE and Bio Re-fuel projects were originally developed at DTU Mechanical Engineering, still a partner in both projects.

Finally, there has been research on carbonate looping in CHEC research centre with collaboration with FLSmidth & Co. A/S coordinated by Associate Professor Weigang Lin. Carbonate looping is a second-generation carbon capture technology, which is especially suitable for the cement industry, where the raw materials can be reacted reversibly between their carbonate form and their oxide form to separate CO_2 from other gases with lower energy penalty.

Experiments and modelling proving the efficiency of the CA-based method have mainly been carried out by Arne Gladis in his PhD project at DTU Chemical Engineering. Arne Gladis was supported by an EU grant through the INTERACT project which also included Professor John Woodley (PROSYS research centre), and after completing his PhD degree, Arne Gladis is now with Wacker Chemie, Germany. The efforts are continued by Postdoc Humbul Suleman, supported by a Eurotech scholarship. Supervisors in both contexts are Associate Professors Nicolas von Solms and Philip L. Fosbøl. The efforts are carried out in collaboration with Novozymes, world-leading supplier of industrial enzymes.

Associate Professor Philip L. Fosbøl and Postdoc Humbul Suleman in the lab.

Philip L. FosbøL
Associate Professor
plf@kt.dtu.dk

Nicolas von Solms
Associate Professor
nvs@kt.dtu.dk

Sludge—from problem to resource

Sprung from DTU Chemical Engineering, start-up company AquaGreen sees sludge from waste water treatment as a resource rather than an environmental problem.

Waste water treatment, aquacultures, and production of biogas all have sludge as a waste fraction. In principle, the sludge can be used directly as fertilizer in agriculture, but complaints from neighbours over smell as well as content of substances which may be problematic for the environment and human health continue to raise concerns. Collaboration between the CHEC research centre at DTU Chemical Engineering and the young engineering company AquaGreen has developed an alternative: Turning the sludge into thermal energy and fertilizer.

The method builds on a combination of superheated steam-drying and pyrolysis. Pyrolysis is the cleaving of organic compounds by heating under anaerobic conditions.

The process is energy efficient, as the energy content of the sludge is utilized for both the drying and the pyrolytic process which converts the solid part of the sludge into a fertilizer. The end product, known as bio-char, has a high content of nutrients necessary for the growth of plants, espe-

Bio-char from sewage sludge - sustainable phosphorus fertilizer without environmentally harmful substances

"As the bio-char produced in AquaGreen's process has less than 10 per cent volume and weight in comparison to the sludge, you are no longer limited to finding application close to the source."

cially phosphorous. Notably, the content of problematic substances such as pathogenic bacteria and residues from pharmaceutical products—both found in sludge from waste water treatment—has been eliminated in the up to 650° C pyrolytic heating.

Another major advantage is the significantly lower price of transportation.

"Whenever you transport sludge, you are really transporting more than 90 per cent water, which obviously does not contribute to fertilizing. As the bio-char produced in the new process has less than 10 per cent volume and weight in comparison to the sludge, you are no longer limited to finding application close to the source of the sludge," explains Senior Researcher Jesper Ahrenfeldt, DTU Chemical Engineering.

The next challenge: Upscaling
AquaGreen was founded in 2014 based on findings in the group at DTU Chemical Engineering. As a first move, the company targeted the aquaculture sector in Norway. Here, environmental problems had forced local producers to move part of production onshore. This improved water quality in the fiords but also resulted in sludge being produced onshore, creating a market for AquaGreen's technology.

After successful introduction in Norway, the company is now ready to conquer new markets. To this end, the collaboration with the CHEC group—which has been involved all along—will be extended further.

"While the fundamental technology is fully demonstrated and in commercial use, we still need to tackle various chemical engineering issues on the academic side. These are mainly related to upscaling of the processes. In a country like Denmark, waste water treatment is the most interesting application, but this will require building the plants somewhat larger to become economically feasible. As always, upscaling involves chemical engineering challenges. There are still some first-of-a-kind solutions waiting to be developed," says Jesper Ahrenfeldt.

Legislation drives the transformation
Besides waste water treatment, production of biogas is another promising market for the technology. In Denmark, biogas is largely produced from manure and organic household waste. After the gas is produced, sludge remains, still having some 40-50 per cent of the original energy content. This fits in nicely with the AquaGreen technology.

While the technology is proven, several barriers still need to be overcome, Jesper Ahrenfeldt notes:

"The business case relies on farmers being willing to use bio-char. We see interest going up, but also know that agriculture is generally a conservative sector when it comes to introducing new technology and practises."

Recent developments give rise to optimism:

"Germany has banned the direct disposal of sludge in agriculture, and we see similar legislation under way in other European countries. Denmark will surely follow at some point. This will obviously support the argument for using bio-chair instead of sludge, and thereby prompt a wider use of the new technology."

Jesper Ahrenfeldt
Senior Scientist
jeah@kt.dtu.dk


PhD student Spardha Virendra Jhamb and Associate Professor Xiaodong Liang.

Virtual prediction of bio-degradability

Companies striving to improve the sustainability of their products are helped by software developed in the KT Consortium. The project was initiated by industry member Syngenta.

Some companies manufacture products that will unavoidably end up in the environment and should thus preferably be readily biodegradable. Prompted by a member company, Syngenta, researchers in the KT Consortium have developed a new tool able to predict the biodegradability of most new components that a company might consider to use.

"As long as the molecular structure of the compound under consideration is known and fairly simple, we are able to calculate its biodegradability with high accuracy. The uncertainty in the method increases, the more irregular the structure of the new substance is, and the less it resembles known structures," says Associate Professor at DTU Chemical Engineering Xiaodong Liang. He has supervised the development which has been carried out by PhD student Spardha Virendra Jhamb and visiting student Irène Hospital, Université de Lorraine, France.

The tool produces a biodegradability value with two or three decimals, usually in the range from 0 to 1.

Xiaodong Liang further notes that for most practical purposes a company would normally be happy to just know whether the given substance is readily biodegradable (values above 0.5), non-biodegradable (values below 0.2) or somewhere in-between.

May replace costly lab experiments
Owned by ChemChina, Syngenta is a leading provider of agricultural chemicals and seeds, supplying farmers worldwide. The company is committed to improving the sustainability of its products in accordance with the United Nation's Sustainable Development Goals. These efforts involve improving and documenting biodegradability. Here, the idea of building a virtual tool for prediction of the biodegradability properties came up—supplementing or possibly even replacing costly and time-consuming lab experiments.

As Syngenta has been a KT Consortium member for a decade, it was a natural step for the company to approach the group at DTU Chemical Engineering.

"The first communication on the idea took place in January 2018, so development has been fairly rapid," says Xiaodong Liang.

dichromate, providing a measure of the total amount of oxidizable matter present in the sample.

High rate of success
The BOD/COD ratio can be seen as a measure for biodegradability. A 1.00 value would indicate that the compound is fully biodegradable.

With this in place, the next step was to develop a model for biodegradability estimation. The chosen model is based on the so-called group-contribution methods, which are simple, easy to use and widely used in chemical process system engineering.

Finally, results from the model were compared with experimental data derived partly from literature, and partly from Syngenta's extensive database.

"The results are promising, with a regression coefficient of 0.92 and an average absolute error of 0.05, and a 96 per cent success of classifying a compound as 'readily biodegradable" or not,' says Xiaodong Liang.

"The results are promising, with (...) a 96 per cent success of classifying a compound as 'readily biodegradable' or not."

The first challenge was obviously to establish what is meant by the term biodegradable. It was decided to measure the biodegradability of a chemical using a combination of two oxidation parameters.

The first parameter is BOD (Biochemical Oxygen Demand), which is the amount of oxygen demanded by aerobic bacteria when metabolising a test compound. Common practise of labs in many countries have established measuring BOD after five days of incubation at 20°C as a global standard.

COD (Chemical Oxygen Demand) is the amount of oxygen consumed during oxidation of a test compound with hot, acidic

He further notes that the methodology can be applied not only by Syngenta:

"The group-contribution methods are quite general. We will be able to use them for different properties and object functions in other DTU Chemical Engineering projects. Also, we are about to integrate them in our ICAS software (Integrated Computer Aided Systems, the main deliverable from the KT Consortium), thereby allowing other consortium member companies to benefit."

Xiaodong Liang
Associate Professor
xlia@kt.dtu.dk

Improved coatings for fire protection

Improving the sustainability of coatings able to dampen the destructive consequences of a fire is an example of the highly interdisciplinary coatings research at DTU Chemical Engineering.

Coatings for passive fire protection are like airbags in a car. They remain idle for years, but when the accident suddenly takes place, they absolutely need to work. Making these so-called intumescent coatings more sustainable is an example of the complex challenges faced by the researchers at CoaST (The Hempel Foundation Coatings Science and Technology Centre) at DTU Chemical Engineering.

"The main driver here is health concerns. All the many benefits of passive fire protection aside, we have to recognize that the current products do contain substances which have been shown to be carcinogenic or otherwise problematic to human health," says Associate Professor Søren Kiil.

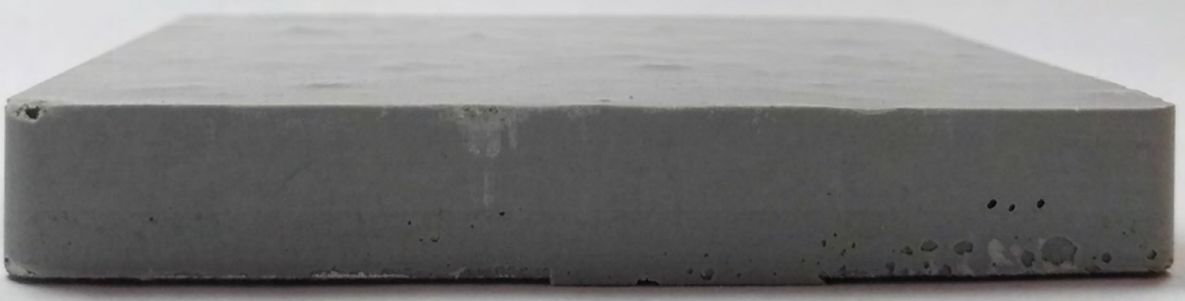
Intumescent coatings are mainly used for steel structures. At elevated temperatures, an intumescent coating will swell by as much as 40 times into a foam which will quickly stiffen and become char. The layer of char is thermally insulating, meaning that the inevitable heating of the steel takes place at a significantly reduced pace. Without this protection, the steel could quickly loose strength leading to collapse of the structure.

Passive fire protection may save lives

Intumescent coatings exist in two classes, one for normal buildings and one for more critical infrastructure like oil rigs. The presence of hydrocarbons triggers more violent fire development. Therefore, coatings for this purpose need to respond faster.

The first intumescent coatings were invented around 100 years ago. Since then, these coatings have been improved in various ways, but the interest in developing more sustainable formulations is relatively new.

An example of a problematic substance found in intumescent coatings is zinc borate. The researchers in CoaST have ideas for less hazardous alternatives. However, the question is



A hydrocarbon intumescent coating with a thickness of 6 mm applied on the surface of a grit-blasted steel plate. The coating is a two-component (base and curing part) epoxy-based system which is targeted specifically at passive fire protection against hydrocarbon fire scenarios.

whether the technical properties will still live up to specifications. At an oil rig, for instance, lives may well depend on intumescent coatings. The coating will not put out the fire, but it will dampen the effects and give personnel time to evacuate.

"We want to develop more environmentally benign coatings, but we cannot compromise safety. We need to be sure that our sustainable alternatives will still function after say 15 or 20 years," says Claus E. Weinell. As Senior Executive Officer he is responsible for experimental facilities in CoaST.

A recent initiative is specially developed table-size electro-ovens for the experiments.

"Traditionally, coatings are tested in big industry-type ovens. We realized that smaller electric ovens would be better for our research. They can be heated up and cooled down much faster than larger ovens. Furthermore, we can obtain better control of the conditions and thus more accurate results. And finally, we simply save energy consumption and costs by doing the experiments in smaller ovens," Claus E. Weinell states.

Accelerated testing is imperative

Obviously, the researchers cannot wait for 15 years to see if the properties are still according to specifications. Therefore, accelerated tests are a key part of their setup. An example is cyclic weathering, where the temperature is raised and lowered repeatedly.

An intumescent char formed in a fire-resistance experiment of a hydrocarbon intumescent coating according to the temperature-time relationship defined in the standard hydrocarbon fire testing curve UL1709. The thickness of the expanded char (55 mm) is nine times the original thickness of the coating (6 mm).

"In this way, we increase the driving forces which create degradation of the coating under real-life circumstances," explains Claus E. Weinell, continuing:

"However, we need to constantly be alert to possible differences between what goes on in the accelerated tests relative to the real situation. We need to understand both the physics and the chemistry involved. This can only be achieved through a constant interplay between experiments, mathematical analysis, modelling and simulations."

Even so, there is still a limit to how much testing can be accelerated:

"If we overdo the accelerated weathering, we will induce phenomena which are different from what is seen in real applications. Therefore, we still need relatively long time spans, typically some months, for the experiments."

Huichao (Teresa) Bi
Assistant Professor
hubi@kt.dtu.dk

Claus E. Weinell
Senior Executive Officer
cwei@kt.dtu.dk

Søren Kiil
Associate Professor
sk@kt.dtu.dk

Real-life fouling and corrosion tests

Recently, a new facility has been added to the experimental portfolio of CoaST. At Hundested, the CoaST researchers are able to operate rafts which can be subjected to real-life fouling and corrosion.

"It is quite unusual for a university to operate a real-life test facility like this," says Assistant Professor Huichao Bi. As a corrosion expert in CoaST, she will use advanced microscopy to spot early signs of degradation in coating-protected steel surfaces.

"We are among the very few people in the world who have applied this technique—Scanning Acoustic Microscopy (SAM)—for the coatings study. Importantly, based on this, we are developing methods which are non-destructive for the coatings performance evaluation, meaning we will be able to study the same samples repeatedly and follow the propagation of failures over time," says Huichao Bi.

Highlights **2019**

20 JANUARY

STUDY TRIP VISIT FROM THE NETHERLANDS

25 students from our partner university TU Eindhoven visited DTU Chemical Engineering and Hempel to learn about this partnership and about study life at campus.

24 JANUARY

TOPPING OUT EVENT

With the topping-out ceremony of Building 228A, DTU Chemical Engineering celebrated a major milestone at the beginning of the year. The new building consists of laboratories, offices, a lounge, as well as an expansion of the existing pilot hall—all carefully placed throughout the 6,000 m^2 of space. Building 228A is expected to be inaugurated in 2021.

22 MARCH

DPC ANNUAL POLYMER DAY

The Annual Polymer Day at Danish Polymer Center was held at Coloplast in Humlebæk to mark the completion of the grant received by Ole Hassager in 2014 from Coloplast—Aage-Louis Hansens Legat. The event had more than 120 participants from DTU Chemical Engineering, Coloplast, the industry, and international universities.

28 MARCH

GEORGIOS M. KONTOGEORGIS RECEIVES ERC ADVANCED GRANT

Professor Georgios M. Kontogeorgis received the ERC Advanced Grant 2018 from the European Research Council for his project "New Paradigm in Electrolyte Thermodynamics". The project aims to create a new paradigm, which will ultimately pave the way for the development of new engineering models for electrolyte solutions.

1-2 APRIL

COAST 2ND ANNUAL DAY AND 1ST WORKSHOP

83 participated in the Annual Day, of which 41 were industrial partners. PhD students and postdoc fellows presented their projects and results within the field of coatings. The workshop had 22 participants of which 3 represented international academia.

1 MAY

MARINE CENTRE AT HUNDESTED HARBOUR

On 1 May, the raft used in Roskilde Fjord in a former PhD fouling control research project was transported to Hundested harbour to get a revival. During May, the raft was modified and finally launched in Hundested harbour on 28 May. Based on experience from 2019, a much larger facility will be established next year.

15 MAY

EXPERIENCED ASSOCIATE PROFESSOR'S ANNIVERSARY CELEBRATED

Associate Professor Weigang Lin celebrated his 25-year anniversary at the CHEC research centre at DTU Chemical Engineering's facilities. Weingang Lin has been instrumental in developing the fruitful cooperation between DTU Chemical Engineering and Institute of Process Engineering, CAS, in China.

8-10 JUNE

CERE DISCUSSION MEETING

Modelling the behaviour of electrolytes in energy resources engineering has always been tricky. At the CERE Discussion Meeting 2019, members of the CERE industry Consortium appreciated the academic efforts to address this issue.

12-14 JUNE

KT CONSORTIUM ANNUAL MEETING

KT Consortium Annual Meeting 2019 was attended by 70 participants of whom 17 were representatives of member companies and one from academia. At the meeting, several industry representatives pointed to the value of the ICAS software—one of the main KT-Consortium deliverables, combining computer-aided tools for modelling, simulation, property prediction, synthesis/design, control, and analysis into a single integrated system—in their quest for improved sustainability.

30 JUNE

MICETECH PROJECT SUCCESSFULLY CONCLUDED

The advanced technology platform 'Minerals and Cement Process Technology—MiCeTech' funded by the Innovation Fund Denmark, FLSmidth A/S, Hempel and DTU was concluded successfully. The platform, which started in 2013, has resulted in important scientific and business results within the three main research areas: Cement processes, minerals processes, and coatings. Further, the platform has facilitated tight cooperation among the partners and recruitment of new employees from the project in both partner companies. A strong basis for future cooperation has been created.

2-3 JULY

THIRD KT-IPE SEMINAR

For years, the Danish-Chinese cooperation has resulted in joint education in the framework of SDC and research that benefit the sustainable development for Denmark and China. In early July, the leadership of DTU Chemical Engineering and the Institute of Process Engineering, Chinese Academy of Sciences came together in Marienlyst for the third joint seminar to further consolidate the collaboration and facilitate cooperative projects within sustainable energy, green processes, and advanced materials and formulated products.

12 JULY

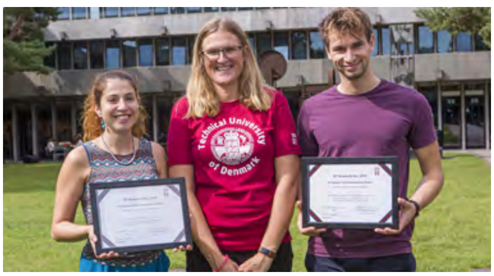
GÜRKAN SIN WINS HUTCHISON MEDAL

The IChemE Hutchison Medal 2018/2019—awarded for both practical and wide-ranging, philosophical or thought-provoking published papers—has been awarded to a scientific paper involving Associate Professor Gürkan Sin as a co-author.

Highlights **2019**

23-30 AUGUST
7TH BIOPRO WORLD TALENT CAMPUS
The advanced one-week course at PhD level organized by the BIOPRO consortium was held for 25 PhD students from all over the world. The focus was on biomanufacturing, including topics such as on-line measurement techniques, mathematical modelling and control of bio-based processes.

29 AUGUST
BIG GRANT PAVES THE WAY FOR INTERNATIONAL COOPERATION
The Novo Nordisk Foundation granted DKK 182.7 million to an international partnership between DTU and North Carolina State University (NCSU) aimed at the establishment of new biopharmaceutical processes and study programmes for students and employees in the industry. The collaboration will involve both DTU Chemical Engineering and DTU Bioengineering.



30 AUGUST
RESEARCH DAY 2019
Focus this year was on the key developments within the Department and the industry, and Head of DTU Entrepreneurship, Professor Jes Broeng gave an inspiring talk entitled Research-based Entrepreneurship. The winners of this year's highly successful PhD video workshop—PhD students Valeria Chiaula and Frederik Zafiryadis—were found on this occasion. The workshops have become an increasingly popular initiative to help the PhDs communicate their research in the digital age.

9-13 SEPTEMBER
2ND INTERNATIONAL EUROMBR TRAINING COURSE - INNOVATIVE MICROBIOREACTOR APPLICATIONS IN BIOPROCESS DEVELOPMENT
The International EUROMBR Training Course originates from the Marie Curie Initial Training Network EUROMBR coordinated by DTU Chemical Engineering and financed by the FP7 of the European Union. Within this network, application-oriented professionals from nine countries have been working together for the education, development and application of the explorative MBR technology to sustain the future progress of biobased processes. With the EUROMBR Training Course, the EUROMBR consortium makes its expertise accessible to all prospective scientists who want to gain a deeper understanding of microbioreactor technology. In 2019, 35 young researchers have been participating at this course, held at the Center of Pharmaceutical Engineering (PVZ), Technische Universität Braunschweig, Germany, including also lectures by Associate Professor Ulrich Krühne.

2 OCTOBER
GIRLS DAY IN SCIENCE
In AT CERE, girls from local high schools were invited to workshops in the DTU Chemical

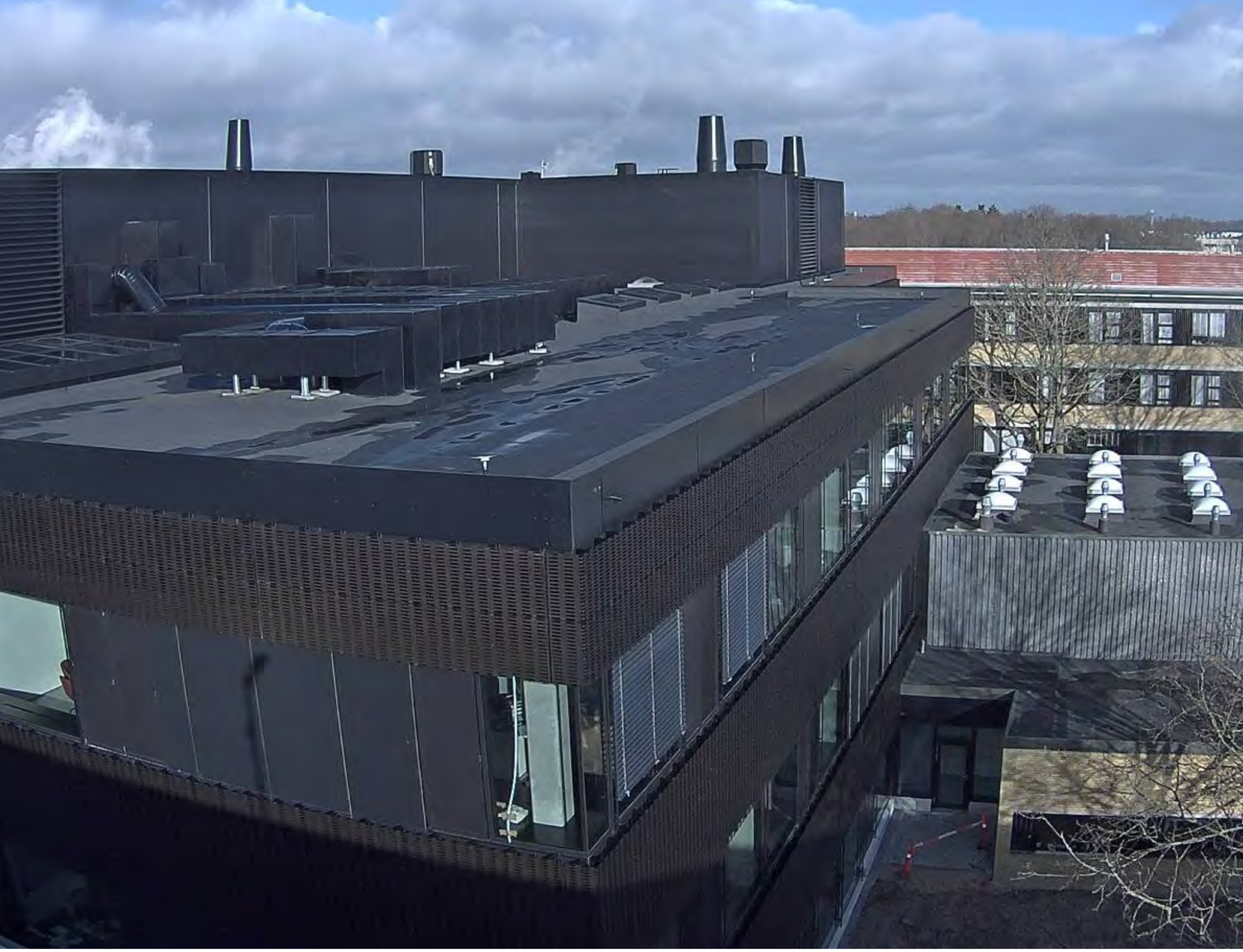
Engineering laboratories to get a close-up experience of scientific work for the annual Danish Girls Day in Science. This year, the high schoolers were investigating some of the climate solutions needed to meet the global challenges of the future.

25 OCTOBER
PROSYS ANNUAL RESEARCH SEMINAR
The seminar, with guest speakers from Freesense ApS, Novo Nordisk, and Pall Corporation, gave its 110 participants the opportunity to learn about the ongoing projects within PROSYS, and also to meet and discuss in an informal way with the PhD students, postdocs, senior researchers, and faculty members of the centre during the poster sessions. Furthermore, the seminar was, as always, an opportunity for our industrial stakeholders to connect with colleagues across different industries.

29 NOVEMBER
INNOEXPLORER GRANT
Professor Anne Ladegaard Skov and her DPC team received an InnoExplorer grant from Innovation Fund Denmark for the project Glysious. This is a spinout in the making from DTU Chemical Engineering that created a silicone adhesive with glycerol domains embedded that release active substances while ensuring the right humidity level in the wound bed.

12 AND 15 NOVEMBER
VISIT FROM HIGH SCHOOLS
The science students from Odense Technical High School visited the department for the second time. Already in 2015, they won the Hempel-DTU Award for science high schools, which included a trip to DTU Chemical Engineering. But they wanted another visit this year, as their Production Technology classes were working with the themes chemical production and food products. Also, this year's winners visited DTU to get an introduction to the life of an engineering student. The Award is a way for the Hempel Foundation and DTU to strengthen the science work at high schools.

6 DECEMBER
SHARING INNOVATIVE IDEAS
As the year was waning, the entire Department gathered to celebrate the annual Christmas seminar. On the agenda was innovation. Former Associate Professor at DTU Chemical Engineering Tue Johannessen was invited to give a talk on innovation in chemical engineering. As co-founder of Amminex Emissions Technology A/S and now Senior Innovation Portfolio Manager at A.P. Møller–Mærsk A/S Tue gave inspiring examples on how to approach innovation from different perspectives. In addition, each centre gave a presentation on their respective takes on innovation and examples on how they implement them in their work.




BJARNE VEJLE
PETZL

NEW

SURROUNDINGS FOR A NEW DECADE

2019 was truly a year of transformation for DTU Chemical Engineering. Our new 6,000-m^2 Building 228A was completed and put to use in 2020. The new building symbolizes a modern university anno 2020 with cross-function cooperation between research, teaching, and administration.

The new facilities include laboratories for both research and teaching as well as an expansion of our existing pilot plant with large-scale experiments. With the large and modernized expansion, the Department is be able to meet current and future demands for teaching and research and to continue innovating and teaching in even better conditions.

We look forward to the formal inauguration—an event where we will also celebrate the last 150 years of technical chemistry at DTU and the many benefits this have had and still has on society.

Building a community on fermentation

The interest in Fermentation Based Biomanufacturing is on the rise in chemical, pharmaceutical and biotech industries. A new cross-departmental effort at DTU will deliver candidates and PhDs with the exact profile required.

In an industrial context, fermentation is the manufacture by any of a variety of organisms—bacteria, yeasts, fungi, cell cultures—of desired products, which could be chemicals, enzymes, proteins, etc. Spanning across three departments at DTU, a research-based programme takes education and training in Fermentation Based Biomanufacturing (FBM) to a new level. The programme is designed to create candidates with both a deep knowledge of biology, deep knowledge on scaling up, pilot operations and strong mathematical and programming skills.

"We are fulfilling a long-standing wish from industry. Traditionally, a university graduate would either be keen on biotechnology or on chemical engineering. In FBM you need to have an understanding of both worlds. This is what we offer," explains Professor John Woodley, DTU Chemical Engineering.

The FBM education is based on cutting-edge research covering all aspects of fermentation, e.g. fundamental physiology of production organisms, metabolic engineering, scale-up processes, and downstream processing.

Overall coordination lies with DTU Bioengineering, while DTU Chemical Engineering and the Novo Nordisk Foundation Center for Biosustainability are the two other partners.

Industry standard level of containment

Each year at DTU Chemical Engineering, two PhD students will be hired at FBM. The first three are already onboard, while the hiring process for the next ones is ongoing. Further, some 15-20 students from the Departments will do their master projects under the FBM umbrella every year.

The research facilities at DTU Chemical Engineering play a key role in the programme.

"The rapid development in fermentation-based biomanufacturing means that we can rarely use all the content from past years' courses. Still, this is also what is so thrilling about working in this field."

"We already have excellent pilot plant facilities, and with the upcoming inauguration of the new Building 228A, these facilities will be upgraded further. Not least a new fermentation plant with 300 L fermenter (around 200 L working volume) production capacity will allow us to do experiments at a useful scale en route to industry," says John Woodley, noting that the pilot facility will be classified as 'GMO 1'—the standard containment level in Danish industry.

"Importantly, we will not just have the equipment itself, but mirror all components digitally. These 'Digital Twins' will have a dual function. They will be important in our teaching, and also contribute to research projects, improving our understanding of what is going on during the fermentation and downstream operations."

Lifelong learning in digital formats

The new initiative can already claim great interest—no less than 120 students signed up for the first of the new master's courses during the fall semester of 2019.

"To see this level of interest is really great. It is also quite demanding in terms of the amount of teaching we have to deliver—not least since the rapid development in fermentation-based biomanufacturing means that we can rarely use all the content from past years' courses. Still, this is also what is so thrilling about working in this field," John Woodley comments.

The FBM initiative involves several training programmes.

"The concept of lifelong learning is highly relevant to FBM, as technology and fundamental understanding progress so rapidly. Therefore, it is a natural part of our activity to provide courses for industry staff and other candidates. Some of these courses will be offered in digital formats, and we plan to extend these options further," says John Woodley.

Expansion in digitalization and downstream processing

The high level of activity has already prompted the involved DTU departments to hire additional scientific staff. At DTU Chemical Engineering, Assistant Professor Helena Junicke has become faculty member, while a faculty member at professorial level is due to be recruited in 2020.

"Also, we plan to hire new postdocs to assist us in research, not least with a focus on digitalization and downstream processing," John Woodley informs.

With the FBM initiative, industry is well on track to get its wish granted for a new type of candidates and PhDs with both biological and chemical engineering skills.

"Maybe even more important is the fact that the field has become stronger and more visible here at DTU," John Woodley notes. "The three departments involved each have their strongholds, and by getting closely aligned in this way, we are able to grow a healthy community on fermentation based biomanufacturing—something also highly appreciated by our industry partners."

The FBM Initiative

Backed by a donation from the Novo Nordisk Foundation, the FBM (Fermentation Based Biomanufacturing) initiative is scheduled to run for the coming five years. It will continue for another two years after that, as the initiative includes a PhD programme—and the PhD students starting towards the end of the five-year period will of course be able to complete their projects, normally running for three years.

The FBM industry partners are Bioneer, Chr. Hansen, AGC Biologics, Dupont, Glycom, Novo Nordisk, Novozymes, and Xelia. The companies take part in teaching and offer internships to master students.

John Woodley
Professor
jw@kt.dtu.dk

How can we make plastic more sustainable?

All stages of plastics use, from processing to initial product and after-life will need to be taken into account for design of tomorrow's plastic materials and to increase their value for society.

The optimal sustainable polymer would be made from biological feedstock and be fully recyclable. However, we cannot get to this ideal scenario in one go, as Anders E. Daugaard, Associate Professor with the Danish Polymer Centre (DPC) at DTU Chemical Engineering, explains:

"We still see more bio-based polymers with satisfactory technical properties being developed. This is good news for climate change mitigation. We need alternative sources of raw materials, and production of bio-based polymers does emit less CO_2 than production of polymers from fossil raw materials. However, these bio-polymers do not recycle well so far. I would argue that a fossil polymer, such as our current commodity plastics, which can be recycled many times, is in fact more sustainable than a bio-based polymer that can only be used once."

Further, Anders E. Daugaard wants us to think polymer sustainability in a broader context:

"We should not only be concerned about the source of raw material or the fate of the polymer itself, but also include its function. Without polymer wrapping, food like fish, meat, and fruit would quickly go bad. We would have to return to the situation 50 years ago, where people had to do most of their shopping at a daily basis. And we would waste a lot more food than we currently do. This would hardly be sustainable."

Multi-layer foils challenge recycling

Most consumers don't know that as they pick up a random tray with fresh meat at the supermarket, the product is protected not by one, but typically 5-7 different layers of foil. The middle layer will have excellent barrier properties—stopping meat juice from getting out, and oxygen from getting in—while the other layers add other technical properties.

"The result is unique protection, and we can thus see food products last for several weeks rather than maybe a couple of days. However, from a recycling perspective this

"A fossil polymer, such as our current commodity plastics, which can be recycled many times, is in fact more sustainable than a bio-based polymer that can only be used once."

is really problematic. It is just not possible to separate these 5-7 different layers after collection. At the very best, you may be able to tolerate these polymers in a blended form in granulated re-used polymer, which could be utilized for making, say, an outdoor bench. Nevertheless, you will never be able to restore the excellent barrier properties and re-use these high-value polymers for the original purpose," says Anders E. Daugaard.

Solving this problem will require a combination of technical research and a change of attitude, Anders E. Daugaard argues:

"Efforts in many research groups, including ours, aim at developing novel polymers which as one-layer foils have satisfactory barrier and other properties. This will enable recycling for the original purpose. We have shown that a significant improvement can be achieved using various composite systems. Such solutions are able to meet requirements in some areas of packaging. However, even though a lot of progress is made, it is still very difficult to meet the excellent barrier properties of the best multi-layer foils."

Through a recently granted Innovation Fund Denmark Grand solutions project, DPC will collaborate with industrial partners covering all the elements of processing and preparation of industrial solutions to reduce the need for muli-layer foils for packaging applications.

Getting value out of plastic waste at all stages of the process

Reducing plastic consumption during processing by direct recirculation, when possible, or through industrial recycling is currently being done. However, for some materials, such as multi-layer foils or thermosets, this is particularly difficult, since these cannot just be re-grinded and recirculated into the production. In these cases, companies will not even be able to recycle waste created in-house.

"We're talking about significant quantities here, and it should be possible to utilize this resource. Multi-layer foils are one such example, but also thermoset materials or heavily degraded materials that have been in circulation, are fractions that will need to be handled, says Anders E. Daugaard"

If a quantum of newly produced polymer has some kind of flaw, it will often have to be incinerated. In addition to waste from production, also thermoset materials as well as heavily degraded or mixed plastics need to be recycled to a much greater extent to generate higher value from these types of materials.

Through an internal collaboration at the Department, we combine gasification technology from the CHEC research group with our expertise on plastics, together with industrial and academic partners in an Innovation Fund Denmark Grand Solutions project, to extract higher value products from such complicated waste fractions. Particularly, the possibility to be able to produce new pristine polymers from these raw materials holds a great potential for increasing the value of these waste fractions.

"By considering all the stages of plastics use, from processing to initial product and after-life, we believe it will be possible to both reduce the amount of waste as well as to increase the value of the waste products that we as a society will inevitably create. All of these aspects are critical in the development of a more sustainable use of plastics, Anders E. Daugaard concludes".

Anders E. Daugaard
Associate Professor
adt@kt.dtu.dk

Microbes make tricky biomass useful

Turning residual biomass into a resource rather than waste has previously been difficult. A novel process produces methane with very high yield.

Lignocellulosic biomasses, organic household waste, waste from food industries, and pig manure are the main raw materials in the growing Danish biogas industry. However, some 40-50 per cent of the energy content is still present in the residual sludge after the biogas has been produced. A new process developed in an interdisciplinary project involving several groups at DTU Chemical Engineering is able to convert biomass into methane with very high carbon efficiency: Close to 100 per cent of the carbon present in the raw materials ends up in the methane. Methane is a valuable fuel and has the further advantage of being storable in the already established Danish infrastructure for natural gas.

As a first step, the biomass is converted into 'syngas'—which is a mixture of H_2, CO_2, and CO—through gasification. This is a commercially available process. However, syngas in itself is not an ideal product.

"While syngas is used for instance as a resource for combined heat and power production, this involves a number of practical challenges, since the syngas cannot be stored and has to be used when it is produced," Associate Professor Ioannis V. Skiadas explains.

"By pairing the combined heat and power production with the fermentation of syngas, the processing of residual biomasses can always follow the optimum path. That is, the production will be easily diverted to either combined heat or power, or to storable biofuels, thus satisfying the supply and demand of the biomass and energy markets at the given time."

A microbial process is the key

When the demand for heating and electricity is high, the syngas may be exploited mainly through combined heat and power, but when the heating and electricity demand is low, the syngas will be fermented to storable biofuels like methane. The fermentation takes place at atmospheric pressure and very mild temperatures (30 - 60 °C), and therefore it is very simple and comes with very low operational costs. This makes the technology particularly suitable for relatively small gasification plants, which is the usual case for Denmark.

Therefore, the real novelty in the project is the proven ability to process the syngas further into methane using fermentation, which is a microbial process.

A number of industrial fermentation processes rely on pure microbial cultures where a single microbial species is used—often in a genetically engineered version—to perform a very specific task. For instance, this is a common strategy in the pharmaceutical industry. In contrast, the fermentation in this project at DTU Chemical Engineering is based on mixed microbial consortia.

"Pure cultures require costly procedures, for instance sterilizing equipment and feedstock, to avoid contamination from other species. This can be justified if you manufacture a high value product like an active pharmaceutical ingredient, but for a product like methane you need something cheaper," Associate Professor Hariklia N. Gavala explains.

However, using mixed microbial consortia is not just hoping for the best. The team has developed enriched microbial cultures for this specific purpose.

Pilot reactor is in operation
Another factor which strongly contributes to the close to 100 per cent methane yield, is the development of thermodynamically driven enrichment processes and reactor operations, not least a trickle bed reactor. This has helped to further develop the process to include hydrogen (which can be produced with renewable electricity from wind turbines) and biologically convert the remaining CO_2 content of the gases into methane as well.

Proof-of-concept for the reactor has been achieved in a lab-scale version, and a 30 times up-scaled pilot version is now in operation—both with close to 100 per cent methane yield.

In practice, any type of biomass will be relevant, Ioannis V. Skiadas explains:

"This could be straw, wood pellets, residual sludge from biogas production, etc. Whenever you have a bio-resource that is rich in carbon and poor in water, gasification into syngas will be possible."

Next step: Higher value chemicals
Further, production of methane could be just the first step in utilization of tricky biomass resources, Hariklia N. Gavala notes:

"We have also shown the possibility to produce ethanol and other chemicals from mixed microbial consortia. This could be an even more promising utilization of the difficult biomass fractions, as these chemicals have higher value than methane. "

A new enabling technology has been the development of combined biomimetic membranes and diabatic distillation for the purification of the produced ethanol.

"The next step will be implementation in industry, possibly at a biogas, combustion, or gasification facility. We hope to attract interest from one or more companies as soon as we have the final report ready," says Associate Professor Jens Abildskov.

The project has created a general overview of existing and new technologies.

"We have managed to create an innovative benchmarking study, for recovery of ethanol as an example of a higher value chemical. The project clearly shows how energy use can be reduced by applying the right know-how. We have also improved the understanding of reactor design which will reduce the size of future full-scale plants," concludes Associate Professor Philip Fosbøl.

The SYNFERON project

The gasification/bio-conversion technology platform for production of methane and possibly other chemicals has been developed at DTU Chemical Engineering in the SYNFERON project (Optimised SYNgas FERmentatiON for biofuels production).

Partners in the SYNFERON project are DTU Chemical Engineering, Danish Gas Technology Centre, Aquaporin A/S, Biosystemer ApS, Highterm Research GmBH (Germany), and Bioeconomy Institute at Iowa State University (USA). Of the initial total budget of EUR 2.8 million, EUR 2.3 million was financed by Innovation Fund Denmark, while the partners have contributed with the remaining EUR 0.5 million. Professor Georgios M. Kontogeorgis, DTU Chemical Engineering, was overall coordinator.

The SYNFERON project was formally completed by summer 2019, but efforts and collaborations continue with the aim of implementing the developed technology platform.

At DTU Chemical Engineering, the SYNFERON project has been highly interdisciplinary involving staff from the AT CERE centre, the PROSYS centre, and the Pilot Plant.

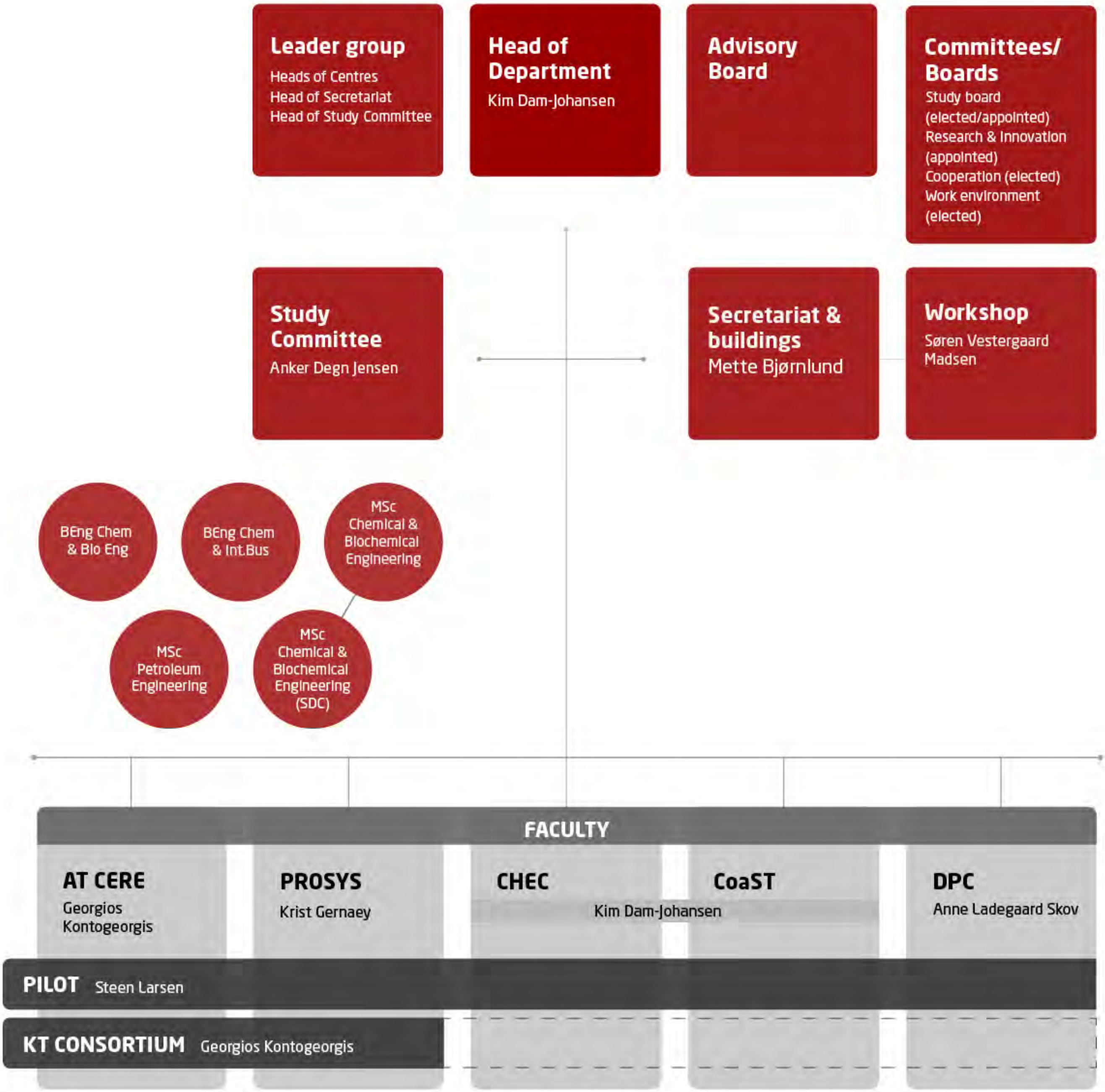
Ioannis V. Skiadas
Associate Professor
ivsk@kt.dtu.dk

Hariklia N. Gavala
Associate Professor
hnga@kt.dtu.dk

Jens Abildskov
Associate Professor
ja@kt.dtu.dk

Philip L. Fosbøl
Associate Professor
plf@kt.dtu.dk

Organization



Research centres

DTU Chemical Engineering is home to five research centres, one cross departmental Pilot Plant facility and one industry-academia collaboration—each focusing on their area of expertise. Below you can get a quick overview of the centres and facilities and their respective research areas.

AT CERE

In Applied Thermodynamics—Center for Energy Resources Engineering (AT CERE), we focus on applied thermodynamics, transport processes and properties, mathematical modelling, materials science, petroleum technology, enhanced oil recovery, CO_2 capture, and gas hydrates and energy resources.

CHEC

In Combustion and Harmful Emission Control (CHEC), we focus on catalysis, inorganic chemistry, combustion and flue gas cleaning, diagnostics, gasification, pretreatment of biomass, and pharmaceutical production.

DPC

At Danish Polymer Center (DPC), we focus on polymer technology based on deep knowledge on polymer chemistry, rheology, filament stretching rheology, surface modification, silicone polymers, and elastomers.

COAST

The focal points in The Hempel Foundation Coatings Science and Technology Centre (CoaST) are sustainable coatings technologies including raw material engineering, smart formulation and production principles, application, testing and tailor-made functionalities.

PILOT PLANT

The cross-departmental Pilot Plant facility focuses on designing and building large-scale plants to perform, teach and develop unit operations, industrial chemical processes, operational experience, design of components, plant safety, and good manufacturing practice.

PROSYS

Process and Systems Engineering Centre (PROSYS) is focused on developing state-of-the-art Process Systems Engineering (PSE) methods and tools, as well as to develop and demonstrate novel technologies for future more sustainable production processes, including industrial fermentation technology, biocatalysis and downstream processing.

KT CONSORTIUM

KT Consortium is an industry-academia collaboration where members are provided networking opportunities and state-of-the-art methods and tools for chemical and biochemical engineering. Faculty and researchers from two of the Department's centres, AT CERE and PROSYS, participate in KT Consortium.

To learn more about our research, recent results, or current projects, please visit **www.kt.dtu.dk/research.**

The Faculty **2019**

SCIENTIFIC

Alexander Shapiro
Associate Professor

Anders E. Daugaard
Associate Professorr

Anne Ladegaard Skov
Professor

Anker D. Jensen
Professor

Georgios Kontogeorgis
Professor

Gürkan Sin
Associate Professor

Hao Wu
Associate Professor

Hariklia N. Gavala
Associate Professor

Helena Junicke
Assistant Professor

Huichao (Teresa) Bi
Assistant Professor

Ioannis V. Skiadas
Associate Professor

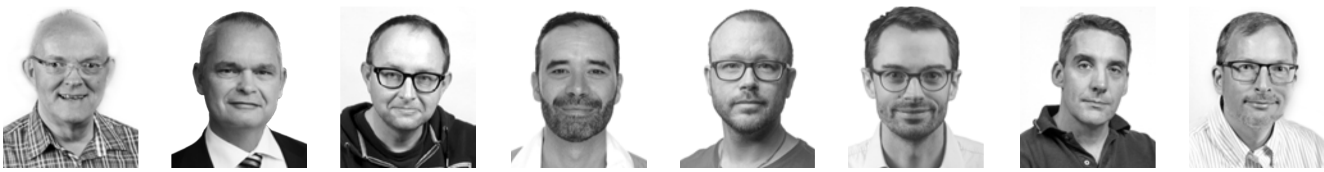
Jakob K. Huusom
Associate Professor

Jakob M. Christensen
Associate Professor

Jens Abildskov
Associate Professor

Jesper Ahrenfeldt
Senior Scientist

John Woodley
Professor



Kaj Thomsen
Associate Professor

Kim Dam-Johansen
Professor,
Head of Department

Krist V. Gernaey
Professor

Manuel Pinelo
Associate Professor

Martin Andersson
Associate Professor

Martin Høj
Assistant Professor

Nicolas von Solms
Associate Professor

Peter Szabo
Associate Professor

Peter Glarborg
Professor

Philip L. Fosbøl
Associate Professor

Seyed S. Mansouri
Assistant Professor

Stig Wedel
Associate Professor

Søren Kiil
Associate Professor

Ulrich Krühne
Associate Professor

Xiaodong Liang
Associate Professor

ADMINISTRATIVE AND OPERATIVE

Mette Bjørnlund
Head of Secretariat

Ivan Hundebøl
Special Consultant,
PILOT PLANT

Khosrow Bagherpour
Senior Consultant
PILOT PLANT

Steen Larsen
Head of PILOT PLANT

EMERITUS

Gunnar E. Jonsson
Associate Professor
Emeritus

Hanne Østergård
Emeritus

John Villadsen
Professor Emeritus

Lars G. Kiørboe
Emeritus

Ole Hassager
Professor Emeritus

Sten B. Jørgensen
Professor Emeritus

Advisory Board

LARS BANG
EXECUTIVE VICE PRESIDENT,
H. LUNDBECK A/S

"Implementing manufacturing of new medicines and continuously exploiting innovative new technologies to optimize manufacturing is key to the competitiveness of Lundbeck. Through a long-term partnership with DTU Chemical Engineering, we are working together with a world-class research group. It has significantly increased our technological competences and capabilities. At the same time it has improved our network and thereby the basis for attracting the right new engineers to drive further progress."

THOMAS VIDEBÆK
CHIEF OPERATING OFFICER,
NOVOZYMES A/S

"At Novozymes, we aim at finding biological answers, for better lives, in a growing world. Fermentation technology holds enormous potential and every day we work together with partners around the world to improve chemical processes. Thereby reducing the need for scarce resources for the benefit of consumers, our partners, as well as the planet."

BJERNE CLAUSEN
PRESIDENT & CHIEF
EXECUTIVE OFFICER,
HALDOR TOPSØE A/S

"Topsøe's solutions within catalysis help solve some of the world's most serious challenges. In order to develop our products and meet future needs, our close partnership with DTU Chemical Engineering is indispensable. We aim for the same high scientific and quality standards, and in Topsøe we are greatly inspired by the remarkable knowledge, drive, and curiosity of the students and candidates from DTU Chemical Engineering."

LARS PETERSSON
PRESIDENT & CHIEF
EXECUTIVE OFFICER,
HEMPEL A/S

"At Hempel, we strive every day to solve the challenges of our customers by providing coating solutions which protect their assets, lower their impact on the environment, and enhance their performance. In that quest for solutions, DTU Chemical Engineering is an invaluable partner for us to tap into the latest research within the fields of formulations, processes, and sustainability. Cooperating with DTU Chemical Engineering also creates an excellent opportunity for attracting talent and developing future and existing Hempel employees."

HANNE EVERLAND
VICE PRESIDENT TECHNOLOGY,
GLOBAL R&D, COLOPLAST A/S

"The best results are never achieved alone. For Coloplast, performance and collaboration go hand in hand. Working together with colleagues, customers, and partners, we share knowledge and explore new possibilities. That's what moves things from what they are, to what they could be. It is our mission to always be at the forefront of new technology and innovation within medical devices for people with intimate healthcare needs and therefore we have this partnership with DTU Chemical Engineering. The polymer research and education as an integrated part of Chemical Engineering is important not only for Coloplast, but for the medical device industry in Denmark in general."

Cooperating companies

A
Addifab
Akzo Nobel
Alfa Laval
Aquagreen
Aquaporin
ARKEMA FRANCE
AstraZeneca
AVEVA Software

B
Babcock & Wilcox Vølund
Basewater
BP
Burkert
BW Scandinavian Contractor

C
Calsep
Centro Tecnológico Componentes
Chempilots
Chevron
Coloplast
Contura
Covestro Deutschland AG

D
DSM
DuPont Nutrition and Biosciences Denmark

E
EnCoat
Equinor
ExxonMobil

F
Firmenich SA
FLSmidth
Fluidan

G
GEA Process Engineering
Gelest
GlaxoSmithKline
Grundfos

H
Haldor Topsøe
Hempel
Hess
HOFOR
Hundested Havn
Hwam

I
I/S Vestforbrænding
IFP

J
Janssen pharmaceutical company of Johnsson & Johnson

K
Kalundborg forsyning A/S
KBC

L
LEAP Technology
LEGO
LeoPharma
Linde
LiqTech International
Logstor
Lundbeck
Lundsby Biogas

M
Madsen Bioenergi
MAN Energy Solutions
Microsoft
Mitsubishi
MOL Group
Multiflex-folien
Mölnlycke

N
National Oilwell Varco
NEO GROUP
Neptune Energy
Neste Jacobs Oy
Nordic Sugar
Nouryon
Nova Pangeae
Novo Nordisk
Novozymes

P
ParticleTech
Petrobras
Pharmacosmos
Process Design
Processi Innovativi SRL
Processium
ProSim SA

Q
Q-Interline

R
Radiometer
Rambøll Danmark
Rockwool

S
Schlumberger
Shell
Sinopec
SYNESIS
Syngenta

T
TOTAL

U
Umicore Denmark
Unibio Group
Unilever
Union Engineering

W
Welltec
Wintershall

X
Xellia Pharmaceuticals

Y
Ystral

Ø
Ørsted

On 4 February 2019, KTStudents visited Ørsted's Avedøre Power Station (Avedøreværket) in Hvidovre.

KTStudents: Connecting with industry

As a multicultural student organization that holds both professional and social events for the students at the Department, KTStudents not only creates bonds between students, but also connects students and the industry.

2019 was a busy year for KTStudents. The student organization visited companies such as Ørsted, SPX Flow and Dutch Nystar as well as Eindhoven Technical University.

"Through these activities, we would like to create a better learning environment for our fellow students, where the students can discover more about their future career options while having a good time with their friends at the Department," says chairman of KTStudents Hsi Tsao.

The students visited Ørsted's Avedøre Power Station. They interacted with a chemical engineer working there and had a tour around the power station where they could ask questions and get to know more about the energy company.

For the spring semester, KTStudents has already planned to visit CP Kelco, Chr. Hansen and Fujifilm.

"We are constantly trying to grow our connections with the industry and provide our fellow students more opportunities to interact with the industry," says Hsi Tsao.

Contact KTStudents on KTSO@kt.dtu.dk

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 2018-31 AUGUST 2019

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 in chemical engineering
28923	Uncertainty and sensitivity analysis of numerical models
28927	Advanced topics in process technology
28928	Electrolyte solutions 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
88708	Green chemical engineering
88709	Fluidization and multiphase flow
88710	Combustion and high temperature processes
88711	Industrial bioreaction engineering
88713	SDC Green Challenge
88714	SDC summer school in unit operations
88715	Biorefinery
88716	Coatings science and technology

Courses

MSC, BSC, AND BENG COURSES

Below, course numbers and names are shown for 2018-2019, 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 (68)
28012 Chemical and biochemical process engineering (91) **(B)**
28016 Mathematical models for chemical and biochemical systems (94) **(B)**
28020 Introduction to chemical and biochemical engineering (61)
28022 Unit operations of chemical engineering and biotechnology (94) **(B)**
28121 Chemical unit operations laboratory (26)
28125 Chemical unit operations laboratory (22)
28140 Introduction to chemical reaction engineering (38)
28150 Introduction to process control (70)
28157 Process and product design (46) **(B)**
28213 Polymer technology (45)
28233 Recovery and purification of biological products (71)
28242 Chemical kinetics and catalysis (65)
28244 Combustion and high temperature process (55)
28310 Chemical and biochemical product design (54)
28315 Colloid and surface chemistry (60)
28316 Laboratory course in colloid and surface chemistry (19)
28322 Chemical engineering thermodynamics (82) **(B)**
28342 Chemical reaction engineering (54) **(B)**
28344 Biotechnology and process design (28) **(B)**
28352 Chemical process control (37) **(B)**
28420 Separation processes (71)
28515 Enhanced oil recovery (13)
28530 Transport processes (66)
28831 Computational fluid dynamics in chemical engineering (20)
28845 Chemical reaction engineering laboratory (19)
28852 Risk assessment in chemical industry (56)
28864 Introduction to Matlab programming (45)
28870 Energy and sustainability (102)
28872 Biorefinery (56)

Courses given in cooperation with other departments:

23522 Rheology of food and biological materials (19)
26010 Introductory project in chemistry (68)
36004 Health, diseases and technology (61)
41683 Materials science (26) **(B)**

SPRING-SEMESTER

28012 Chemical and biochemical process engineering (33) **(B)**
28016 Mathematical models for chemical and biochemical systems (30) **(B)**
28020 Introduction to chemical and biochemical engineering (59)
28022 Unit operations of chemical engineering and biotechnology (42) **(B)**
28025 Bio process technology (82)
28121 Chemical unit operations laboratory (9)
28157 Process design (40) **(B)**
28160 Mathematical models for chemical systems (44)
28212 Polymer chemistry (45)
28214 Polymer synthesis and characterization (12)
28221 Chemical engineering thermodynamics (43)
28231 Laboratory in chemical and biochemical engineering (13)
28322 Chemical engineering thermodynamics (24) **(B)**
28342 Chemical reaction engineering (50) **(B)**
28344 Biotechnology and process design (57) **(B)**
28345 Chemical reaction engineering (41)
28346 Advanced fermentation technology practicum (15)
28350 Process design: Principles and methods (56)
28352 Chemical process control (44) **(B)**
28361 Chemical engineering model analysis (72)
28415 Oil and gas production (23)
28423 Phase equilibria for separation processes (12)
28434 Membrane technology (54)
28443 Industrial reaction engineering (31)
28451 Optimizing plantwide control (34)
28535 Rheology of complex fluids (light) (0)
28811 Polymers in processes and products (10)
28850 Quality by design (QbD): Integration of product and process development (85)
28855 Good manufacturing practice (103)
28864 Introduction to Matlab programming (48)
28871 Production of biofuels (27)
28885 Technology and economy of oil and gas production (13) **(B)**

Courses given in cooperation with other departments:

12701 Introduction to living systems (73)
26317 Instrumental chemical analysis (48)
41683 Materials science (68) **(B)**

BACHELOR OF ENGINEERING DEGREES

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

Biomethanation of syngas in mesophilic and thermophilic trickle-bed bioreactors
Characterization of Norwegian farmhouse microbial cultures for beer production
Characterisation of the degradation of heterogeneous catalysts in upflow reactors
Chromatographic separation
Continuous oxidation of phosphorous rich biochar
Cost estimation API manufacture by solid phase peptide synthesis
Crystallization in continuous flow
Design and analysis of small scale photobioreactors for cultivation of microalgae
Design of a pilot scale setup for bubble size examination **(2 students)**
Development and validation of a mini parallel fed-batch reactor setup for rapid bioprocess design
Development of a method for production of Dextran T20
Development of high flux forward osmosis hollow fiber membranes **(2 students)**
Development of high retention forward osmosis hollow fiber membranes
Development of methods for immobilized lipase pressure-drop measurements
Development of procedure for wood particle pyrolysis experiments
Drop tube study of urea decomposition
Dynamic analysis of an industrially validated simulation model
Feasibility study on non-destructive strength measurement on 7 hole tablets
Flexible rubber coating
Frost on bulk bags and breached bags: A potential source of cross and hygiene contaminations at Chr. Hansen
Image analysis software module development for determination of size distributions of small objects
In-situ monitoring of fast evolving particles in emulsions by using continuous image analysis
Modeling and simulation of processes with salt solutions
Modeling methylamine oxidation
Multi-reactor laboratory scale-down system for bioprocess characterization and optimization
Optimisation of insulin APX processes
Optimising the recovery of ammonia from aqueous ammonia soaked biomass in a pilot scale test unit
Periodic separation
Pilot study of the potential of Aquaporin inside TM forward osmosis membrane to concentrate xenobiotics in municipal wastewater effluent
Porcine trypsin: Process mapping and yield optimization
Process optimization based on mapping and risk analysis of production processes at Nohrlund Organic Cocktails **(2 students)**
Qualification and process validation of ultrafiltration setup for immunoglobulin purification
Recovery process economics and inventory optimization
Separation of chiral lactic acids **(2 students)**
Simulation of chemical and biochemical production processes
Systematic downstream process synthesis, design and analysis for butanol production
Thermodynamic modeling of industrial salt system

BACHELOR OF SCIENCE DEGREES

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

Advanced regulatory control of the Tennessee Eastman process
Application of spectroscopy techniques for real-time monitoring of fermentation processes
Automatization of iterative heat exchanger design
Developing an interactive mathematical model to predict gradients and required mass transfer in a U-loop fermentor
Drug delivery from silicone-glycerol elastomers
Dynamic and non-linear polymer rheology
Enzymatic synthesis of DFF from HMF using galactose oxidase
Establishing robust temperature and pH regulation on a pilot scale U-loop reactor
Flue gas cleaning by membrane separation **(2 students)**

Investigation of alternative molybdates for selective catalytic oxidation of methanol to formaldehyde
Investigation of catalytic decomposition of glycolaldehyde **(2 students)**
Investigation of close-coupled SCR for automotive exhaust gas cleaning for NO_x
Investigation of the catalytic oxidation of methane in the presence of SO_2
Measurement and model of reaction kinetics for new solvents in CO_2 capture
Measurement of properties of CO_2 capture solvent
Nano structuring of silicone elastomers for optical applications
Preparation and modelling of chain extended silicone networks
Syngas conversion to ethanol over rhodium-based catalysts
Synthesis and analysis of ionic liquid as additive for Li-ion battery electrolyte
Systematic tuning of PID controllers in non-steady-state wastewater treatment systems
Thermodynamic modeling of aqueous salt system
Thermodynamic modelling of associating compounds for gas processing

MASTER OF SCIENCE DEGREES

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

Analysis of rinsing solvents and optimization of purification processes for 3D printed objects
Analyzing process operation constraints in industrial spray drying
Anti-corrosive coating degradation evaluation under marine environment conditions
Aqueous Ammonia Soaking, AAS for pre-treatment of lignocellulosic biomasses: Potential for methane enhancement and ammonia recovery
Benchmarking cathode materials of commercial and industrial relevance for sodium-ion batteries
Biomass-degrading enzyme discovery from marine microorganisms for macroalgae decomposition
CO_2 storage by hydrate swapping - flooding and CT scanning
Computational fluid dynamic investigation of a static mixer in a pilot scale U-loop reactor
Computer based industrial enzyme design
Control of divided wall distillation columns
Corrosion and coating breakdown—comparison between real life and accelerated laboratory testing
Cyclic separations
Data driven compartment modelling of bioreactors using free-floating sensors
Decomposition of urea
Design and simulation of rate-based CO_2 absorption processes
Design, construction, and measurement of CO_2 capture in a mini pilot
Designing biotech facilities of the future
Development and optimisation of an industrial process for hydrolysis of sucrose
Development of a coking model for catalyst deactivation during the methanol to gasoline reaction
Enzymatic esterification of free fatty acids in crude biodiesel using continuous bubble reactor system
Enzymatic esterification of free fatty acids in crude biodiesel using stepwise flash for water removal
Experimental analysis of CO_2 vapour liquid equilibrium on solvent for biogas upgrading
Experimental determination and modelling of reaction kinetics for condensation curing silicone coatings
Experimental investigation of a water jet CIP cleaning device
Experimental investigation of CH_4-CO_2 swapping in gas hydrates **(2 students)**
Extensional rheology of polymer melts
Feasibility study on energy recovery from brewers spent grains
FCA-controlled nutrient addition during microbial fermentations
Fermentation of syngas to methane in trickle bed bioreactors: Lab and pilot scale
Gas phase conversion of glycolaldehyde to new chemicals
Hardening process of protective coating systems
Hardness build-up in polyurethane top coats
Immobilization of MAO for continuous operation
Immobilized enzymes on thin-film composite reverse osmosis membranes for fouling mitigation
Impact of ultrasonic sound on CO_2 reboiler desorption performance
In situ measurement of absorbed dose in irradiated polymer material and medical devices made therefrom

Integration of various polymeric nanostructures incorporating Aquaporin Z protein into the active layer of biomimetic membranes
Integrated process/product design
Influence of TiO_2 crystal defects on automotive V-SCR
Investigation of cross-linking effect on proteopolymersome reconstituting Aquaporin Z proteins
Modelling and design studies of the crystallization step in the biotechnological production process of xylitol
Modeling of salt precipitation from industrial brines
Model based capacity analysis, production planning-scheduling of an API production utility blending process
Model based capacity analysis for an insulin product
Model-based control analysis and simulation of a pharmaceutical recovery process
Model-based development of control strategies for mitigating greenhouse gas emissions from wastewater treatment plants
Model-based dynamic simulation and control of a solvent recovery process
Model for urea decomposition
Nanomechanical properties of microgels and polymer layers
New screening assay for coating process optimization and testing
Optimization of growth and expression conditions for the production of selected aquaporins in S. cerevisiae
Periodic separation control
Pneumatic transport of bulk solids
Polyhydroxyalkanoates production from concentrated fermented effluents: Effect of VFA and 1.3 PDO concentration
Predictive modelling for production of catalyst with a view to plantwide control **(2 students)**
Preparation of polymer solutions for 3D printing
Process intensification for in-situ removal of inhibitors
Pyrolysis and oxidation kinetics of binders used in stone wool products
Pyrolysis of bio-dust
Reactor development for GOX biocatalysis
Read length optimization of nanopore MinION sequencing data
Renewable biofuel process design using hydrotreatment of vegetable oil
Rheology of highly filled polymer matrices
Screening of optimum process conditions for butanol production in mixed microbial cultures
Simultaneous material and process optimization of adsorption processes for H_2 purification and CO_2 capture
Simulation based methods for engineering optimization
Synergetic effect of fillers on the performance of hydrocarbon intumescent coatings
Synthesis and characterization of thermoplastic elastomers used for pressure sensitive adhesive formulations for skin applications
Solvent design for chromatographic separation
Tailoring and optimization of matrix properties and interactions between enzymes and support materials
The influence of additives on deposit formation from biomass combustion **(2 students)**

SDC MASTER'S DEGREES

12 students finished their research projects for the MSc Degree/Double degree. The project titles are listed below:

An EMMS-based flow regime study. Focusing on high-density circulating fluidized beds
Application research of enzymatic membrane reactor to produce fructose dextrose syrup
Butene dimerization catalyzed by acidic ionic liquids
Controllable synthesis of VPO catalysts: Optimization of synthesis conditions
Design and preparation of bimetallic nanocomposites supported on porous carbon derived from biomass and its application in catalysis
Ionic liquid-based composite membranes for CO_2 separation
Step-wise condensation in coal pyrolysis process for fractional of coal tar
Study on gasification technology of municipal sludge
Study on structure control and electrochemical performance of $Li_4TI_5O1_2$ anode material
The study on the catalytic hydrogenation of CO_2 to synthesize C_2 oxygenated chemicals
Theoretical study on the structure-interaction relationship of long chain ionic liquid-amino acid system
Using bio-electrochemical systems (BESs) to produce methane

WoS publications

Aghaalikhani, Arash; Schmid, Johannes C.; Borello, Domenico; Fuchs, Joseph; Benedikt, Florian; Hofbauer, Herman; Rispoli, Franco; Henriksen, Ulrick B.; Sárossy, Zsuzsa; Cedola, Luca / **Detailed modelling of biomass steam gasification in a dual fluidized bed gasifier with temperature variation**. Renewable Energy, Vol. 143, 2019, pp. 703-718.

Al, Resul; Behera, Chitta Ranjan; Zubov, Alexandr; Gernaey, Krist V.; Sin, Gürkan / **Meta-modeling based efficient global sensitivity analysis for wastewater treatment plants – An application to the BSM2 model**. Computers & Chemical Engineering, Vol. 127, 2019, pp. 233-246.

Anane, Emmanuel; López C, Diana C.; Barz, Tilman; Sin, Gürkan; Gernaey, Krist V.; Neubauer, Peter; Cruz Bournazou, Mariano N. / **Output uncertainty of dynamic growth models: Effect of uncertain parameter estimates on model reliability**. Biochemical Engineering Journal, Vol. 150, 2019, pp. 1-12.

Ang, Teck N.; Udugama, Isuru A.; Mansouri, Seyed S.; Taylor, Matthew; Burrell, Rob; Young, Brent R.; Baroutian, Saeid / **A techno-economic-societal assessment of recovery of waste volatile anaesthetics**. Separation and Purification Technology, Vol. 226, 2019, pp. 304-314.

A. Udugama, Isuru; Alvarez Camps, Martina; Taube, Michael A.; Thawita, Chatchayarat; Anantpinijwatna, Amata; Mansouri, Seyed Soheil; Young, Brent R.; Yu, Wei / **A novel soft sensor for measuring and controlling recovery in a high-purity, multi-component, side-draw distillation column**. Industrial & Engineering Chemistry Research, Vol. 58, No. 43, 2019, pp. 20026-20035.

Baehner, Franz D.; Huusom, Jakob K. / **A Debottlenecking Study of an Industrial Pharmaceutical Batch Plant**. Industrial & Engineering Chemistry Research, Vol. 58, No. 43, 2019, pp. 20003-20013.

Bähner, Franz D.; Santacoloma, Paloma A.; Huusom, Jakob K. / **Assessment of the Plantwide Control Structure in a Pectin Production Plant**. IFAC-PapersOnLine, Vol. 52, No. 1, 2019, pp. 251-256.

Bähner, Franz D.; Santacoloma, Paloma A.; Huusom, Jakob K. / **Optimal operation of parallel dead-end filters in a continuous bio-based process**. Food and Bioproducts Processing, Vol. 114, 2019, pp. 263-275.

Barrett, Kristian; Lange, Lene / **Peptide-based functional annotation of carbohydrate-active enzymes by conserved unique peptide patterns (CUPP)**. Biotechnology for Biofuels, Vol. 12, No. 102, 2019, pp. 1-21.

Bentil, Joseph A.; Thygesen, Anders; Lange, Lene; Mensah, Moses; Meyer, Anne S. / **Green seaweeds (*Ulva fasciata* sp.) as nitrogen source for fungal cellulase production**. World Journal of Microbiology and Biotechnology, Vol. 35, No. 82, 2019, pp. 1-8.

Bjerregaard, Matias F.; Charalampidis, Angelos; Frøding, Rasmus; Shetty, Radhakrishna; Pastell, Helena; Jacobsen, Charlotte; Zhuang, Shiwen; Pinelo, Manuel; Hansen, Preben B.; Hobley, Timothy J. / **Processing of brewing by-products to give food ingredient streams**. European Food Research and Technology, Vol. 245, No. 3, 2019, pp. 545-558.

Cabaneros Lopez, Pau; Feldman, Hannah; Mauricio-Iglesias, Miguel; Junicke, Helena; Huusom, Jakob K.; Gernaey, Krist V. / **Benchmarking real-time monitoring strategies for ethanol production from lignocellulosic biomass**. Biomass and Bioenergy, Vol. 127, 2019, pp. 1-14.

Cai, Jing; Tao, Yuan-Qing; von Solms, Nicolas; Xu, Chun-Gang; Chen, Zhao-Yang; Li, Xiao-Sen / **Experimental studies on hydrogen hydrate with tetrahydrofuran by differential scanning calorimeter and in-situ Raman**. Applied Energy, Vol. 243, 2019, pp. 1-9.

Camacho Vergara, Edgar L.; Kontogeorgis, Georgios M.; Liang, Xiaodong / **Gas Adsorption and Interfacial Tension with Classical Density Functional Theory**. Industrial & Engineering Chemistry Research, Vol. 58, No. 14, 2019, pp. 5650-5664.

Capellades, Gerard; Duso, Alessandro; Dam-Johansen, Kim; Mealy, Michael J.; Christensen, Troels V.; Kiil, Søren / **Continuous Crystallization with Gas Entrainment: Evaluating the Effect of a Moving Gas Phase in an MSMPR Crystallizer**. Organic Process Research & Development, Vol. 23, No. 2, 2019, pp. 252-262.

Caroço, Ricardo F.; Kim, Boeun; Santacoloma, Paloma A.; Abildskov, Jens; Lee, Jay H.; Huusom, Jakob K. / **Analysis and model-based optimization of a pectin extraction process**. Journal of Food Engineering, Vol. 244, 2019, pp. 159-169.

Caroço, Ricardo F.; Bevilacqua, Marta; Armagan, Ibrahim; Santacoloma, Paloma A.; Abildskov, Jens; Skov, Thomas; Huusom, Jakob K. / **Raw material quality assessment approaches comparison in pectin production**. Biotechnology Progress, Vol. 35, No. 2, 2019, pp. 1-13.

Chatterjee, Rishika; Kuld, Sebastian; van den Berg, Roy; Chen, Aling; Shen, Wenjie; Christensen, Jakob M.; Jensen, Anker D.; Sehested, Jens / **Mapping Support Interactions in Copper Catalysts**. Topics in catalysis, Vol. 62, 2019, pp. 649-659.

Chen, Xueming; Lai, Chun-Yu; Fang, Fang; Zhao, He-Ping; Dai, Xiaohu; Ni, Bing-Jie / **Model-based evaluation of selenate and nitrate reduction in hydrogen-based membrane biofilm reactor**. Chemical Engineering Science, Vol. 195, 2019, pp. 262-270.

Chen, Xueming; Mielczarek, Artur T.; Habicht, Kirsten; Andersen, Mikkel H.; Thornberg, Dines; Sin, Gurkan / **Assessment of Full-Scale N_2O Emission Characteristics and Testing of Control Concepts in an Activated Sludge Wastewater Treatment Plant with Alternating Aerobic and Anoxic Phases**. Environmental Science & Technology, Vol. 53, No. 21, 2019, pp. 12485-12494.

Chen, Xueming; Ni, Bing-Jie; Sin, Gürkan / **Nitrous oxide production in autotrophic nitrogen removal granular sludge: A modeling study**. Biotechnology and Bioengineering, Vol. 116, No. 6, 2019, pp. 1280-1291.

Chen, Xueming; Sin, Gürkan; Ni, Bing-Jie / **Impact of granule size distribution on nitrous oxide production in autotrophic nitrogen removal granular reactor**. Science of the Total Environment, Vol. 689, 2019, pp. 700-708.

Chen, Xueming; Yang, Linyan; Sun, Jing; Dai, Xiaohu; Ni, Bing-Jie / **Modelling of simultaneous nitrogen and thiocyanate removal through coupling thiocyanate-based denitrification with anaerobic ammonium oxidation**. Environmental Pollution, Vol. 253, 2019, pp. 974-980.

Chen, Yuqiu; Gani, Rafiqul; Kontogeorgis, Georgios M.; Woodley, John M. / **Integrated ionic liquid and process design involving azeotropic separation processes**. Chemical Engineering Science, Vol. 203, 2019 pp. 402-414.

Chen, Yuqiu; Kontogeorgis, Georgios M.; Woodley, John M. / **Group Contribution Based Estimation Method for Properties of Ionic Liquids**. Industrial and Engineering Chemistry Research, Vol. 58, No. 10, 2019, pp. 4277-4292.

Chen, Yuqiu; Koumaditi, Evangelia; Gani, Rafiqul; Kontogeorgis, Georgios M.; Woodley, John M. / **Computer-aided design of ionic liquids for hybrid process schemes**. Computers and Chemical Engineering, Vol. 130, 2019, pp. 1-17.

Christensen, Line R.; Hassager, Ole; Skov, Anne L. / **Electro-Thermal Model of Thermal Breakdown in Multilayered Dielectric Elastomers**. AIChE Journal, Vol. 65, No. 2, 2019 pp. 859-864.

Cignitti, Stefano; Rodriguez-Donis, Ivonne; Abildskov, Jens; You, Xinqiang; Shcherbakova, Nataliya; Gerbaud, Vincent / **CAMD for entrainer screening of extractive distillation process based on new thermodynamic criteria**. Chemical Engineering Research and Design, Vol. 147, 2019, pp. 721-733.

Coluccio, Maria L.; D'Attimo, Maria A.; Cristiani, Costanza M.; Candeloro, Patrizio; Parrotta, Elvira; Dattola, Elisabetta; Guzzi, Francesco; Cuda, Giovanni; Lamanna, Ernesto; Carbone, Ennio; Krühne, Ulrich; Di Fabrizio, Enzo; Perozziello, Gerardo / **A Passive Microfluidic Device for Chemotaxis Studies**. Micromachines Vol. 10, No. 551, 2019, pp. 1-11.

Cripwell, Jamie T.; Kruger, Francois J.; Burger, Andries J. / **Accounting for cross association in non-self-associating species using a physically consistent SAFT-VR Mie approach**. Fluid Phase Equilibria, Vol. 483, 2019, pp. 1-13.

Dabros, Trine M. H.; Andersen, Mads L.; Lindahl, Simon B.; Hansen, Thomas W.; Høj, Martin; Gabrielsen, Jostein; Grunwaldt, Jan-Dierk; Jensen, Anker D. / **Hydrodeoxygenation (HDO) of Aliphatic Oxygenates and Phenol over NiMo/$MgAl_2O_4$: Reactivity, Inhibition, and Catalyst Reactivation**. Catalysts, Vol. 9, No. 6, 2019, pp. 1-20.

Dabros, Trine M. H.; Kramer, Hendrik; Høj, Martin; Sprenger, Paul; Grunwaldt, Jan-Dierk; Gabrielsen, Jostein; Jensen, Anker D. / **The Influence of Active Phase Loading on the Hydrodeoxygenation (HDO) of Ethylene Glycol over Promoted MoS_2/$MgAl_2O_4$ Catalysts**. Topics in catalysis, Vol. 62, 2019 pp. 752-763.

Dai, Bingye; Zhu, Weiwei; Mu, Liwen; Guo, Xiaojing; Qian, Hongliang; Liang, Xiaodong; Kontogeorgis, Georgios M. / **Effect of the composition of biomass on the quality of syngas produced from thermochemical conversion based on thermochemical data prediction**. Energy and Fuels, Vol. 33, No. 6, 2019, pp. 5253-5262.

Delgove, Marie A. F.; Laurent, Achille-B.; Woodley, John M.; De Wildeman, Stefaan M. A.; Bernaerts, Katrien V.; van der Meer, Yvonne / **A Prospective Life Cycle Assessment (LCA) of Monomer Synthesis: Comparison of Biocatalytic and Oxidative Chemistry**. ChemSusChem, Vol. 12, No. 7, 2019, pp. 1349-1360.

Dias Gomes, Mafalda; Bommarius, Bettina; Anderson, Shelby; Feske, Brent D.; Woodley, John; Bommarius, Andreas / **Bubble Column Enables Higher Reaction Rate for Deracemization of (R,S)-1-Phenylethanol with Coupled Alcohol Dehydrogenase/NADH Oxidase System**. Advanced Synthesis and Catalysis, Vol. 361, No. 11, 2019, pp. 2574-2581.

Dias Gomes, Mafalda; Moiseyenko, Rayisa P.; Baum, Andreas; Jørgensen, Thomas M.; Woodley, John M. / **Use of Image Analysis to Understand Enzyme Stability in an Aerated Stirred Reactor**. Biotechnology Progress, Vol. 35, No. 6, 2019, pp. 1-11.

Dias Gomes, Mafalda; Woodley, John M. / **Considerations when Measuring Biocatalyst Performance**. Molecules, Vol. 24, No. 19, 2019, pp. 1-11.

Dino Adem, Kamil; Alemu Ambie, Demiss; Puig Arnavat, Maria; Henriksen, Ulrik B.; Ahrenfeldt, Jesper; Thomsen, Tobias P. / **First *injera* baking biomass gasifier stove to reduce indoor air pollution, and fuel use**. Aims Energy, Vol. 7, No. 2, 2019, pp. 227-245.

Dittmann, Karen K.; Porsby, Cisse H.; Goncalves, Priscila; Mateiu, Ramona V.; Sonnenschein, Eva C.; Bentzon-Tilia, Mikkel; Egan, Suhelen; Gram, Lone / **Tropodithietic acid induces oxidative stress response, cell envelope biogenesis and iron uptake in Vibrio vulnificus**. Environmental Microbiology Reports, Vol. 11, No. 4, 2019, pp. 581-588.

Dong, Bin; Xia, Zhaohui; Sun, Jing; Dai, Xiaohu; Chen, Xueming; Ni, Bing J. / **The inhibitory impacts of nano-graphene oxide on methane production from waste activated sludge in anaerobic digestion**. Science of the Total Environment, Vol. 646, 2019, pp. 1376-1384.

Dreyer, Jochen A. H.; Poli, Maximilian; Eaves, Nick A.; Botero, Maria L.; Akroyd, Jethro; Mosbach, Sebastian; Kraft, Markus / **Evolution of the soot particle size distribution along the centreline of an *n*-heptane/toluene co-flow diffusion flame**. Combustion and Flame, Vol. 209, 2019, pp. 256-266.

Eriksen, Marie K.; Christiansen, Jesper de C.; Daugaard, Anders E.; Astrup, Thomas F. / **Closing the loop for PET, PE and PP waste from households: Influence of material properties and product design for plastic recycling**. Waste Management, Vol. 96, 2019, pp. 75-85.

Eschenbacher, Andreas; Jensen, Peter A.; Henriksen, Ulrik B.; Ahrenfeldt, Jesper; Ndoni, Sokol; Li, Chengxin; Duus, Jens Ø.; Mentzel, Uffe V.; Jensen, Anker D. / **Catalytic deoxygenation of vapors obtained from ablative fast pyrolysis of wheat straw using mesoporous HZSM-5**. Fuel Processing Technology, Vol. 194, 2019, pp. 1-15.

Eschenbacher, Andreas; Jensen, Peter A.; Henriksen, Ulrik B.; Ahrenfeldt, Jesper; Li, Chengxin; Duus, Jens Ø.; Mentzel, Uffe V.; Jensen, Anker D. / **Deoxygenation of wheat straw fast pyrolysis vapors using HZSM-5, Al_2O_3, HZSM-5/Al_2O_3 extrudates, and desilicated HZSM-5/Al_2O_3 extrudates**. Energy & Fuels, Vol. 33, No. 7, 2019, pp. 6405-6420.

Eschenbacher, Andreas; Jensen, Peter A.; Henriksen, Ulrik B.; Ahrenfeldt, Jesper; Li, Chengxin; Duus, Jens Ø.; Mentzel, Uffe V.; Jensen, Anker D. / **Impact of ZSM-5 Deactivation on Bio-Oil Quality during Upgrading of Straw Derived Pyrolysis Vapors**. Energy and Fuels, Vol. 33, No. 1, 2019, pp. 397-412.

Falco, Francesco C.; Espersen, Roall; Svensson, Birte; Gernaey, Krist V.; Eliasson Lantz, Anna / **An integrated strategy for the effective production of bristle protein hydrolysate by the keratinolytic filamentous bacterium *Amycolatopsis keratiniphila* D2**. Waste Management, Vol. 89, 2019, pp. 94-102.

Fang, Fang; Xu, Run Z.; Huang, Yan Q.; Wang, Su N.; Zhang, Lu L.; Dong, Jin Y.; Xie, Wen M.; Chen, Xueming; Cao, Jia S. / **Production of polyhydroxyalkanoates and enrichment of associated microbes in bioreactors fed with rice winery wastewater at various organic loading rates**. Bioresource Technology, Vol. 292, 2019, pp. 1-9.

Feldman, Hannah; Flores-Alsina, Xavier; Ramin, Pedram; Kjellberg, Kasper; Jeppsson, Ulf; Batstone, Damien J.; Gernaey, Krist V. / **Assessing the effects of intra-granule precipitation in a full-scale industrial anaerobic digester**. Water Science and Technology, Vol. 79, No. 7, 2019, pp. 1327-1337.

Flores-Alsina, Xavier; Feldman, Hannah; Monje, Vincente T.; Ramin, Pedram; Kjellberg, Kasper; Jeppsson, Ulf; Batstone, Damien J.; Gernaey, Krist V. / **Evaluation of anaerobic digestion post-treatment options using an integrated model-based approach**. Water Research, Vol. 156, 2019, pp. 264-276.

Foerst, Petra; Melo de Carvalho, Teresa; Lechner, Martin; Kovacevic, Tijana; Kim, Seongshik; Kirse, Christoph; Briesen, Heiko / **Estimation of mass transfer rate and primary drying times during freeze-drying of frozen maltodextrin solutions based on x-ray μ-computed tomography measurements of pore size distributions**. Journal of Food Engineering, Vol. 260, 2019, pp. 50-57.

Frutiger, Jérôme; Cignitti, Stefano; Abildskov, Jens; Woodley, John M.; Sin, Gürkan / **Computer-aided molecular product-process design under property uncertainties – A Monte Carlo based optimization strategy**. Computers & Chemical Engineering, Vol. 122, 2019, pp. 247-257.

Gadsbøll, Rasmus Ø.; Clausen, Lasse R.; Thomsen, Tobias P.; Ahrenfeldt, Jesper; Henriksen, Ulrik B. / **Flexible TwoStage biomass gasifier designs for polygeneration operation**. Energy, Vol. 166, 2019, pp. 939-950.

Gadsbøll, Rasmus Ø.; Vivar Garcia, Adrian; Ahrenfeldt, Jesper; Henriksen, Ulrik B. / **Solid oxide fuel cell stack coupled with an oxygen-blown TwoStage gasifier using minimal gas cleaning**. Renewable Energy, Vol. 139, 2019, pp. 1255-1262.

Garg, Nipun; Woodley, John M.; Gani, Rafiqul; Kontogeorgis, Georgios M. / **Sustainable solutions by integrating process synthesis-intensification**. Computers & Chemical Engineering, Vol. 126, 2019, pp. 499–519.

Gaur, Abhijeet; Schumann, Max; Raun, Kristian V.; Stehle, Matthias; Beato, Pablo; Jensen, Anker D.; Grunwaldt, Jan-Dierk; Høj, Martin / **Operando XAS/XRD and Raman Spectroscopic Study of Structural Changes of the Iron Molybdate Catalyst during Selective Oxidation of Methanol**. ChemCatChem, Vol. 11, No. 19, 2019, pp. 4871-4883.

Gaur, Abhijeet; Dabros, Trine M. H.; Høj, Martin; Boubnov, Alexey; Prüssmann, Tim; Jelic, Jelena; Studt, Felix; Jensen, Anker D.; Grunwaldt, Jan-Dierk / **Probing the Active Sites of MoS_2 BasedHydrotreating Catalysts Using Modulation Excitation Spectroscopy**. ACS Catalysis, Vol. 9, No. 3, 2019, pp. 2568-2579.

Ghafarnejad Parto, Soheila; Christensen, Jakob M.; Pedersen, Lars S.; Hansen, Asger B.; Tjosås, Freddy; Spiga, Cristiano; Damsgaard, Christian D.; Larsen, Daniel B.; Duus, Jens Ø.; Jensen, Anker D. / **Liquefaction of Lignosulfonate in Supercritical Ethanol Using Alumina-Supported NiMo Catalyst**. Energy and Fuels, Vol. 33, No. 2, 2019, pp. 1196-1209.

Gladis, Arne; Lomholdt, Niels F.; Fosbøl, Philip L.; Woodley, John M.; von Solms, Nicolas / **Pilot scale absorption experiments with carbonic anhydrase-enhanced MDEA- Benchmarking with 30 wt% MEA**. International Journal of Greenhouse Gas Control, Vol. 82, 2019, pp. 69-85.

Godo-Pla, Lluís; Emiliano, Pere; Valero, Fernando; Poch, Manel; Sin, Gürkan; Monclús, Hèctor / **Predicting the Oxidant Demand in Full-Scale Water Treatment using an Artificial Neural Network: Uncertainty and Sensitivity Analysis**. Process Safety and Environmental Protection, Vol. 125, 2019, pp. 317-327.

Gooya, Reza; Silvestri, Alessandro; Moaddel, Arash; Andersson, Martin P.; Stipp, Susan L. S.; Sørensen, Henning O. / **Unstable, Super Critical CO_2-Water Displacement in Fine Grained Porous Media under Geologic Carbon Sequestration Conditions**. Scientific Reports, Vol. 9, No. 1, 2019, pp. 1-9.

Gunarathne, Duleeka S.; Udugama, Isuru A.; Jayawardena, Sanjivani; Gernaey, Krist V.; Mansouri, Seyed S.; Narayana, Mahinsasa / **Resource recovery from bio-based production processes in developing Asia**. Sustainable Production and Consumption, Vol. 17, 2019, pp. 196-214.

Hammershøi, Peter S.; Godiksen, Anita L.; Mossin, Susanne; Vennestrøm, Peter N. R.; Jensen, Anker D.; Janssens, Ton V. W. / **Site selective adsorption and relocation of SO_x in deactivation of Cu-CHA catalysts for NH_3-SCR**. Reaction Chemistry & Engineering, Vol. 4, No. 6, 2019, pp. 1081-1089.

Hao, Jiasheng; Mohammadkhani, Samira; Shahverdi, Hamidreza; Esfahany, Mohsen Nasr; Shapiro, Alexander / **Mechanisms of smart waterflooding in carbonate oil reservoirs - A review**. Journal of Petroleum Science and Engineering, Vol. 179, 2019, pp. 276-291.

Hartmann, Nanna B.; Hüffer, Thorsten; Thompson, Richard C.; Hassellöv, Martin; Verschoor, Anja; Daugaard, Anders E.; Rist, Sinja; Karlsson, Therese; Brennholt, Nicole; Cole, Matthew; Herrling, Maria P.; Hess, Maren C.; Ivleva, Natalia P.; Lusher, Amy L.; Wagner, Martin / **Are We Speaking the Same Language? Recommendations for a Definition and Categorization Framework for Plastic Debris**. Environmental Science & Technology, Vol. 53, No. 3, 2019, pp. 1039-1047.

Hartmann, Nanna B.; Hüffer, Thorsten; Thompson, Richard C.; Hassellöv, Martin; Verschoor, Anja; Daugaard, Anders E.; Rist, Sinja; Karlsson, Therese; Brennholt, Nicole; Cole, Matthew; Herrling, Maria P.; Hess, Maren C.; Ivleva, Natalia P.; Lusher, Amy L.; Wagner, Martin / **Response to the Letter to the Editor Regarding Our Feature "Are We Speaking the Same Language? Recommendations for a Definition and Categorization Framework for Plastic Debris"**. Environmental Science and Technology, Vol. 53, No. 9, pp. 4678-4679.

Hashemi, Hamid; Christensen, Jakob M.; Harding, Lawrence B.; Klippenstein, Stephen J.; Glarborg, Peter / **High-pressure oxidation of propane**. Proceedings of the Combustion Institute, Vol. 37, No. 3, 2019, pp. 461-468.

Hashemi, Hamid; Christensen, Jakob M.; Glarborg, Peter / **High-pressure pyrolysis and oxidation of DME and DME/CH_4**. Combustion and Flame, Vol. 205, 2019, pp. 80-92.

Hede, Jonas O.; Fosbøl, Philip L.; Berg, Signe W.; Dahl, Søren / **Container closure integrity testing-method development for freeze-dried products using laser-based headspace oxygen analysis**. PDA Journal of Pharmaceutical Science and Technology, Vol. 73, No. 2, 2019, pp. 170-180.

Hedlund, Frank H.; Pedersen, Jan B.; Sin, Gürkan; Garde, Frits G.; Kragh, Eva K.; Frutiger, Jérôme / **Puncture of an import gasoline pipelin-spray effects may evaporate more fuel than a Buncefield-type tank overfill event**. Process Safety and Environmental Protection, Vol. 122, 2019, pp. 33-47.

Heins, Anna-Lena; Johanson, Ted; Han, Shanshan; Lundin, Luisa; Carlquist, Magnus; Gemaey, Krist V.; Sørensen, Søren J.; Eliasson Lantz, Anna / **Quantitative Flow Cytometry to Understand Population Heterogeneity in Response to Changes in Substrate Availability in Escherichia coli and Saccharomyces cerevisiae Chemostats**. Frontiers in Bioengineering and Biotechnology, Vol. 7, 2019, pp. 1-15.

Heins, Anna-Lena; Lundin, Luisa; Nunes, Inês; Gernaey, Krist V.; Sørensen, Søren J.; Eliasson Lantz, Anna / **The effect of acetate on population heterogeneity in different cellular characteristics of *Escherichia coli* in aerobic batch cultures**. Biotechnology Progress, Vol. 35, No. 3, 2019, pp. 1-14.

Hinton, Zachary R.; Shabbir, Aamir; Alvarez, Nicolas J. / **Dynamics of Supramolecular Self-Healing Recovery in Extension**. Macromolecules, Vol. 52, No. 6, 2019, pp. 2231-2242.

Horsholt, Anders; Christiansen, Lasse H.; Meyer, Knud; Huusom, Jakob K.; Jorgensen, John B. / **A Discontinuous-Galerkin Finite-Element Method for Simulation of Packed Bed Chromatographic Processes**. IFAC-PapersOnLine, Vol. 52, No. 1, 2019, pp. 346-351.

Huang, Qian / **Exploring the mechanism of fracture for entangled polymer liquids in extensional flow**. Physics of Fluids, Vol. 31, No. 8, 2019, pp. 1-8.

Huang, Qian; Ahn, Joongho; Parisi, Daniele; Chang, Taihyun; Hassager, Ole; Panyukov, Sergey; Rubinstein, Michael; Vlassopoulos, Dimitris / **Unexpected Stretching of Entangled Ring Macromolecules**. Physical Review Letters, Vol. 122, No. 20, 2019, pp. 1-6.

Huang, Qian; Rasmussen, Helge K. / **Extensional flow dynamics of polystyrene melt**. Journal of Rheology, Vol. 63, No. 5, 2019, pp. 829-835.

Huang, Yuhong; Zheng, Xianliang; Pilgaard, Bo; Holck, Jesper; Muschiol, Jan; Li, Shengying; Lange, Lene / **Identification and characterization of GH11 xylanase and GH43 xylosidase from the chytridiomycetous fungus, *Rhizophlyctis rosea***. Applied Microbiology and Biotechnology, Vol. 103, No. 2, 2019, pp. 777-791.

Hwangbo, Soonho; Nam, KiJeon; Heo, SungKu; Yoo, ChangKyoo / **Hydrogen-based self-sustaining integrated renewable electricity network (HySIREN) using a supply-demand forecasting model and deep-learning algorithms**. Energy Conversion and Management, Vol. 185, 2019, pp. 353-367.

Ilves, Marit; Kinaret, Pia A. S.; Ndika, Joseph; Karisola, Piia; Marwah, Veer; Fortino, Vittorio; Fedutik, Yuri; Correia, Manuel; Ehrlich, Nicky; Löschner, Katrin; Besinis, Alexandros; Vassallo, Joanne; Handy, Richard D.; Wolff, Henrik; Savolainen, Kai; Greco, Dario; Alenius, Harri / **Surface PEGylation suppresses pulmonary effects of CuO in allergen-induced lung inflammation**. Particle and Fibre Toxicology, Vol. 16, No. 1, 2019, pp. 1-21.

Jamali, Asma; Vinhal, Andre P. C. M.; Behnejad, Hassan; Yan, Wei; Kontogeorgis, Georgios M. / **Comparison of two crossover procedures for describing thermodynamic behavior of normal alkanes from singular critical to regular classical regions**. Fluid Phase Equilibria, Vol. 495, 2019, pp. 33-46.

Jhamb, Spardha; Liang, Xiaodong; Gani, Rafiqul; Kontogeorgis, Georgios M. / **Systematic Model-Based Methodology for Substitution of Hazardous Chemicals**. ACS Sustainable Chemistry & Engineering, Vol. 7, No. 8, 2019, pp. 7652-7666.

Ji, Mingbo; Luo, Jianquan; Wei, Jiang; Woodley, John; Daugaard, Anders E.; Pinelo, Manuel / **Commercial polysulfone membranes pretreated with ethanol and NaOH: Effects on permeability, selectivity and antifouling properties**. Separation and Purification Technology, Vol. 219, 2019, pp. 82-89.

Jones, Mark N.; Forero-Hernandez, Hector; Zubov, Alexandr; Sarup, Bent; Sin, Gürkan / **Splitting Triglycerides with a Counter-Current Liquid-Liquid Spray Column: Modeling, Global Sensitivity Analysis, Parameter Estimation and Optimization**. Processes, Vol. 7, No. 12, 2019, pp. 1-22.

Jones, Mark N.; Frutiger, Jérôme; Ince, Nevin G.; Sin, Gürkan / **The Monte Carlo driven and Machine Learning enhanced Process Simulator**. Computers & Chemical Engineering, Vol. 125, 2019, pp. 324-338.

Jørgensen, Sten B; Lind, Morten; Jensen, Niels / **Functional Modeling View on Product and Process Engineering in Design and Operations**. Industrial and Engineering Chemistry Research, Vol. 58, No. 26, 2019, pp. 11129-11148.

Kalafatakis, Stavros; Skiadas, Ioannis V.; Gavala, Hariklia N. / **Determining butanol inhibition kinetics on the growth of Clostridium pasteurianum based on continuous operation and pulse substrate additions**. Journal of Chemical Technology and Biotechnology, Vol. 94, No. 5, 2019, pp. 1559-1566.

Kamp, Andreas; Ambye-Jensen, Morten; Østergård, Hanne / **Modelling matter and energy flows of local, refined grass-clover protein feed as alternative to imported soy meal**. Ecological Modelling, Vol. 410, 2019, pp. 1-12.

Kang, Kai; Zhu, Shanshan; Liang, Xiaodong; Kontogeorgis, Georgios M.; Wang, Xiaopo./ **High-pressure densities of *n*-decane+o-xylene mixtures: Measurement and modelling**. Fluid Phase Equilibria, Vol. 498, 2019, pp. 1-8.

Kang, Kai; Liang, Xiaodong; Kontogeorgis, Georgios M.; Wang, Xiaopo / **PpT measurements and modelling of (n-decane + m-xylene) mixtures from 293.15 K to 363.15 K at pressures up to 60 MPa**. Journal of Chemical Thermodynamics, Vol. 135, 2019, pp. 107-115.

Karlström, Oskar; Wu, Hao; Glarborg, Peter / **Influence of H_2O on NO formation during char oxidation of biomass**. Fuel, Vol. 235, 2019, pp. 1260-1265.

Kazadi Mbamba, Christian; Lindblom, Erik U.; Flores-Alsina, Xavier; Tait, Stephan; Anderson, Sofia; Saagi, Ramesh; Batstone, Damien J.; Gernaey, Krist V.; Jeppsson, Ulf / **Plant-wide model-based analysis of iron dosage strategies for chemical phosphorus removal in wastewater treatment systems**. Water Research, Vol. 155, 2019, pp. 12-25.

Kim, Boeun; Huusom, Jakob K.; Lee, Jay H. / **Robust Batch-to-Batch Optimization with Scenario Adaptation**. Industrial and Engineering Chemistry Research, Vol. 58, No. 30, 2019, pp. 13664-13674.

Kontogeorgis, Georgios M.; Mattei, Michele; Ng, Ka M.; Gani, Rafiqul / **An integrated approach for the design of emulsified products**. A I Ch E Journal, Vol. 65, No. 1, 2019, pp. 75-86.

Kontogeorgis, Georgios M.; Privat, Romain; Jaubert, Jean-Noël / **Taking Another Look at the van der Waals Equation of State – Almost 150 Years Later**. Journal of Chemical and Engineering Data, Vol. 64, No. 11, 2019, pp. 4619-4637.

Kostrzewska, Malgorzata; Yu, Liyun; Li, Yang; Li, Jiansheng; Wenzell, Berit; Kasama, Takeshi; Skov, Anne L. / **Magnetically activated microcapsules as controlled release carriers for a liquid PDMS crosslinker**. Materials Research Express, Vol. 6, No. 1, 2019, pp. 1-11.

Kruger, Francois; Varsos, Athanasios A.; Kontogeorgis, Georgios M.; von Solms, Nicolas / **High-pressure experimental vapour-liquid-liquid equilibrium measurements and modelling for natural gas processing: Equipment validation, and the system CH_4+nC_6H_{14}+H_2O**. Fluid Phase Equilibria, Vol. 501, 2019, pp. 1-13.

Lange, Lene; Pilgaard, Bo; Herbst, Florian-Alexander; Busk, Peter K.; Gleason, Frank; Pedersen, Anders G. / **Origin of fungal biomass degrading enzymes: Evolution, diversity and function of enzymes of early lineage fungi**. Fungal Biology Reviews,Vol. 33, No. 1, 2019, pp. 82-97.

Lange, Lene; Meyer, Anne S. / **Potentials and possible safety issues of using biorefinery products in food value chains**. Trends in Food Science and Technology, Vol. 84, 2019, pp. 7-11.

Law, Yingyu; Matysik, Artur; Chen, Xueming; Swa Thi, Sara; Ngoc Nguyen, Thi Q.; Qiu, Guanglei; Natarajan, Gayathri; Williams, Rohan B. H.; Ni, Bing-Jie; Seviour, Thomas W.; Wuertz, Stefan / **High Dissolved Oxygen Selection against *Nitrospira* Sublineage I in Full-Scale Activated Sludge**. Environmental Science and Technology, Vol. 53, No. 14, 2019, pp. 8157-8166.

Laxminarayan, Yashasvi; Jensen, Peter A.; Wu, Hao; Jappe Frandsen, Flemming; Sander, Bo; Glarborg, Peter / **Biomass Fly Ash Deposition in an Entrained Flow Reactor**. Proceedings of the Combustion Institute, Vol. 37, No. 3, 2019, pp. 2689-2696.

Lejre, Kasper H.; Glarborg, Peter; Christensen, Henrik; Mayer, Stefan; Kiil, Søren / **Mixed Flow Reactor Experiments and Modeling of Sulfuric Acid Neutralization in Lube Oil for Large Two-Stroke Diesel Engines**. Industrial & Engineering Chemistry Research, Vol. 58, No. 1, 2019, pp. 138-155.

Li, Bing; Udugama, Isuru A.; Mansouri, Seyed S.; Yu, Wei; Baroutian, Saeid; Gernaey, Krist V.; Young, Brent R. / **An exploration of barriers for commercializing phosphorus recovery technologies**. Journal of Cleaner Production, Vol. 229, 2019, pp. 1342-1354.

Li, Fangfang; Bai, Yinge; Zeng, Shaojuan; Liang, Xiaodong; Wang, Hui; Huo, Feng; Zhang, Xiangping / **Protic ionic liquids with low viscosity for efficient and reversible capture of carbon dioxide**. International Journal of Greenhouse Gas Control, Vol. 90, 2019, pp. 1-8.

Li, Tian; Skreiberg, Øyvind; Løvås, Terese; Glarborg, Peter / **Skeletal mechanisms for prediction of NO_x emission in solid fuel combustion**. Fuel, Vol. 254, 2019, pp. 1-10.

Li, Qian; Loy-Benitez, Jorge; Nam, Ki J.; Hwangbo, Soonho; Rashidi, Jouan; Yoo, ChangKyoo / **Sustainable and reliable design of reverse osmosis desalination with hybrid renewable energy systems through supply chain forecasting using recurrent neural networks**. Energy, Vol. 178, 2019, pp. 277-292.

Lillia, Stefano; Bonalumi, Davide; Fosbøl, Philip L.; Thomsen, Kaj; Jayaweera, Indira; Valenti, Gianluca / **Thermodynamic and kinetic properties of NH_3-K_2CO_3-CO_2-H_2O system for carbon capture applications**. International Journal of Greenhouse Gas Control, Vol. 85, 2019, pp. 121-131.

Lindeque, Rowan M.; Woodley, John M. / **Reactor Selection for Effective Continuous Biocatalytic Production of Pharmaceuticals**. Catalysts, Vol. 9, No. 3, 2019, pp. 1-17.

Liu, Min; Ladegaard Skov, Anne; Liu, Sheng-Hui; Yu, Li-Yun; Xu, Zhenliang / **A Facile Way to Prepare Hydrophilic Homogeneous PES Hollow Fiber Membrane via Non-Solvent Assisted Reverse Thermally Induced Phase Separation (RTIPS) Method**. Polymers, Vol. 11, No. 2, 2019, pp. 1-18.

Liu, Xiaoyan; Feilberg, Karen Louise; Yan, Wei; Stenby, Erling Halfdan; Thormann, Esben / **Interactions between apolar, basic and acidic model oils and a calcite surface**. Journal of Dispersion Science and Technology,Vol. 40, No. 11, 2019, pp. 1611-1617.

Liu, Zilong; Rios-Carvajal, Tatiana; Andersson, Martin P.; Ceccato, Marcel; Stipp, Susan L. S.; Hassenkam, Tue / **Ion effects on molecular interaction between graphene oxide and organic molecules**. Environmental Science: Nano, Vol. 6, No. 7, 2019, pp. 2281-2291.

Liu, Xue; Yu, Liyun; Nie, Yi; Skov, Anne L. / **Silicone Elastomers with High-Permittivity Ionic Liquids Loading**. Advanced Engineering Materials,Vol. 21, No. 10, 2019, pp. 1-9.

Loldrup Fosbøl, Philip; Neerup, Randi; Almeida, Susana; Rezazadeh, Amirali; Gaspar, Jozsef; Nesse Knarvik, Anette B.; Enaasen Flø, Nina. / **Results of the fourth Technology Centre Mongstad campaign: LVC testing**. International Journal of Greenhouse Gas Control, Vol. 89, 2019, pp. 52-64.

Lopez-Arenas, Teresa; Mansouri, Seyed S.; Sales-Cruz, Mauricio; Gani, Rafiqul; Pérez-Cisneros, Eduardo S. / **A Gibbs energy-driving force method for the optimal design of non-reactive and reactive distillation columns**. Computers & Chemical Engineering, Vol. 128, 2019, pp. 53-68.

Luo, Hao; Lin, Weigang; Song, Wenli; Li, Songgeng; Dam-Johansen, Kim; Wu, Hao / **Three dimensional full-loop CFD simulation of hydrodynamics in a pilot-scale dual fluidized bed system for biomass gasification**. Fuel Processing Technology, Vol. 195, 2019, pp. 1-10.

Ma, Wenchao; Wenga, Terrence; Frandsen, Flemming J.; Yan, Beibei; Chen, Guanyi / **The fate of chlorine during MSW incineration: Vaporization, transformation, deposition, corrosion and remedies**. Progress in Energy and Combustion Science, Vol. 76, 2019, pp. 1-39.

Marke, Henrik S.; Breil, Martin P.; Hansen, Ernst B.; Pinelo, Manuel; Krühne, Ulrich / **Investigation of the Velocity Factor in a Rotational Dynamic Microfiltration System**. Separation and Purification Technology, Vol. 220, 2019, pp. 69-77.

Marshall, Paul; Leung, Caroline; Gimenez-Lopez, Jorge; Rasmussen, Christian T.; Hashemi, Hamid; Glarborg, Peter; Abian, Maria; Alzueta, Maria U. / **The C_2H_2 + NO_2 reaction: Implications for high pressure oxidation of C_2H_2/NO_x mixtures**. Proceedings of the Combustion Institute, Vol. 37, No. 1, 2019, pp. 469-476.

Masche, Marvin; Puig-Arnavat, Maria; Jensen, Peter A.; Holm, Jens Kai; Clausen, Sønnik; Ahrenfeldt, Jesper; Henriksen, Ulrik B. / **From wood chips to pellets to milled pellets: The mechanical processing pathway of Austrian pine and European beech**. Powder Technology, Vol. 350, 2019, pp. 134-145.

Mazurek, Piotr; Ekbrant, Bjørn E. F.; Madsen, Frederike B.; Yu, Liyun; Skov, Anne L. / **Glycerol-silicone foams - Tunable 3-phase elastomeric porous materials**. European Polymer Journal, Vol. 113, 2019, pp. 107-114.

Mazurek, Piotr Stanislaw; Vudayagiri, Sindhu; Skov, Anne / **How to tailor flexible silicone elastomers with mechanical integrity: a tutorial review**. Chemical Society Reviews, Vol. 48, 2019, pp. 1448-1464.

Meng, Xianglei; Ju, Zhaoyang; Zhang, Suojiang; Liang, Xiaodong; von Solms, Nicolas; Zhang, Xiaochun; Zhang, Xiangping / **Efficient transformation of CO_2 to cyclic carbonates using bifunctional protic ionic liquids under mild conditions**. Green Chemistry, Vol. 21, No. 12, 2019, pp. 3456-3463.

Meyer, Kristian; Huusom, Jakob K.; Abildskov, Jens / **A stabilized nodal spectral solver for liquid chromatography models**. Computers and Chemical Engineering, Vol. 124, 2019, pp. 172-183.

Mirtsou-Xanthopoulou, Chrysoula; Skiadas, Ioannis V.; Gavala, Hariklia N. / **On the Effect of Aqueous Ammonia Soaking Pre-Treatment on Continuous Anaerobic Digestion of Digested Swine Manure Fibers**. Molecules, Vol. 24, No. 13, 2019, pp. 1-11.

Mohammadkhani, Samira; Shahverdi, Hamidreza; Nielsen, Sidsel M.; Nasr Esfahany, Mohsen; Shapiro, Alexander / **Bicarbonate flooding of homogeneous and heterogeneous cores from a carbonaceous petroleum reservoir**. Journal of Petroleum Science and Engineering, Vol. 178, 2019, pp. 251-261.

Molla, Getachew S.; Freitag, Michael F.; Stocks, Stuart M.; Nielsen, Kim T.; Sin, Gürkan / **Solubility Prediction of Different Forms of Pharmaceuticals in Single and Mixed Solvents Using Symmetric Electrolyte Nonrandom Two-Liquid Segment Activity Coefficient Model**. Industrial and Engineering Chemistry Research, Vol. 58, No. 10, 2019, pp. 4267-4276.

Mondejar, Maria E.; Frutiger, Jérôme; Cignitti, Stefano; Abildskov, Jens; Sin, Gürkan; Woodley, John M.; Haglind, Fredrik / **Uncertainty in the prediction of the thermophysical behavior of new halogenated working fluids**. Fluid Phase Equilibria, Vol. 485, 2019, pp. 220-233.

Mortensen, Michella R.; Hashemi, Hamid; Wu, Hao; Glarborg, Peter / **Modeling post-flame sulfation of KCl and KOH in bio-dust combustion with full and simplified mechanisms**. Fuel, Vol. 258, 2019, pp. 1-6.

Mu, Liang; Ramløv, Hans; Søgaard, T. Max M.; Jørgensen, Thomas; de Jongh, Willem A.; von Solms, Nicolas / **Inhibition of methane hydrate nucleation and growth by an antifreeze protein**. Journal of Petroleum Science and Engineering, Vol. 183, 2019, pp. 1-8.

Mussati, Sergio F.; Mansouri, Seyed S.; Gernaey, Krist V.; Morosuk, Tatiana; Mussati, Miguel C. / **Model-Based Cost Optimization of Double-Effect Water-Lithium Bromide Absorption Refrigeration Systems**. Processes, Vol. 7, No. 1, 2019, p. 1-16.

Nakhaei, Mohammadhadi; Wu, Hao; Grévain, Damien; Jensen, Lars S.; Glarborg, Peter; Dam-Johansen, Kim / **CPFD simulation of petcoke and SRF co-firing in a full-scale cement calciner**. Fuel Processing Technology, Vol. 196, 2019, pp. 1-15.

Neerup, Randi; Ståhl, Kenny; Fosbøl, Philip L. / **Solid Solubility in the Aqueous 2-Amino-2-methyl-propanol (AMP) Plus Piperazine (PZ) System**. Journal of Chemical and Engineering Data, Vol. 64, No. 6, 2019, pp. 2423-2428.

Ogliani, Elisa; Skov, Anne L.; A. Brook, Michael. / **Purple to Yellow Silicone Elastomers: Design of a Versatile Sensor for Screening Antioxidant Activity**. Advanced Materials Technologies, Vol. 4, No. 11, 2019, 1-7.

Olajuyin, Ayobami M.; Yang, Maohua; Thygesen, Anders; Tian, Jiangnan; Mu, Tingzhen; Xing, Jianmin / **Effective production of succinic acid from coconut water (*Cocos nucifera*) by metabolically engineered *Escherichia coli* with overexpression of *Bacillus subtilis* pyruvate carboxylase**. Biotechnology Reports, Vol. 24, 2019, pp. 1-7.

Oliveira, Ivo; Meyer, Anne S.; Aires, Alfredo; Afonso, Silvia; Gonçalves, Berta / **Enzymatic Activity and Biochemical Composition in Leaves of Green Bean *(Phaseolus vulgaris* L. cv. *Saxa*) Grown in Almond Shell Substrates**. Waste and Biomass Valorization, Vol. 10, No. 5, 2019, pp. 1223-1229.

Pachitsas, Stylianos; Wedel, Stig; Jensen, Lars S.; Illerup, Jytte B.; Dam-Johansen, Kim / **Experimental evaluation of hydrogen chloride (HCl) absorption by cement raw meals at low temperatures, using fixed-bed tests**. Journal of Environmental Chemical Engineering, Vol. 7, No. 2, 2019, pp. 1-12.

Pachitsas, Stylianos; Jensen, Lars S.; Wedel, Stig; Illerup, Jytte B.; Dam-Johansen, Kim / **Hydrogen chloride (HCl) absorption by raw meal and raw meal compounds, using in-situ HCl generation and TGA-FTIR tests**. Journal of Environmental Chemical Engineering, Vol. 7, No. 1, 2019, pp. 1-4.

Pahija, Ergys; Hui, Chi-Wai / **A systematic study on the effects of dynamic environments on microalgae concentration**. Algal Research, Vol. 42, 2019, pp. 1-5.

Pandey, Jyoti S.; von Solms, Nicolas / **Hydrate stability and methane recovery from gas hydrate through CH_4-CO_2 replacement in different mass transfer scenarios**. Energies, Vol. 12, No. 12, 2019, pp. 1-20.

Pandey, Jyoti S.; Jouljamal Daas, Yousef; Solms, Nicolas von. / **Insights into Kinetics of Methane Hydrate Formation in the Presence of Surfactants**. Processes, Vol. 7, No. 9, 2019, pp. 1-19.

Pang, Kar M.; Jangi, Mehdi; Bai, Xue-Song; Schramm, Jesper; Walther, Jens H.; Glarborg, Peter / **Effects of ambient pressure on ignition and flame characteristics in diesel spray combustion**. Fuel, Vol. 237, 2019, pp. 676-685.

Papadakis, Emmanouil; Huusom, Jakob K.; Abildskov, Jens / **Economic analysis of a horizontal diabatic separation system**. Chemical Engineering Research and Design, Vol. 147, 2019, pp. 709-720.

Peng, Lai; Ngo, Huu H.; Song, Shaoxian; Xu, Yifeng; Guo, Wenshan; Liu, Yiwen; Wei, Wei; Chen, Xueming; Wang, Dongbo; Ni, Bing-Jie / **Heterotrophic denitrifiers growing on soluble microbial products contribute to nitrous oxide production in anammox biofilm: Model evaluation**. Journal of Environmental Management, Vol. 242, 2019, pp. 309-314.

Perzon, Alixander; Muschiol, Jan; Meyer, Anne S.; Munk, Line; Liu, Ming; Holland, Claire; Jørgensen, Bodil; Ulvskov, Peter / **Interaction between feruloylated arabinoxylan and nanocellulose: Effect on bulk rheological and material properties**. American Chemical Society. Abstracts of Papers (at the National Meeting), Vol. 257, No. 255, 2019.

Petersen, Leander A. H.; Lieven, Christian; Nandy, Subir K.; Villadsen, John; Jørgensen, Sten B.; Christensen, Ib; Gernaey, Krist V. / **Dynamic investigation and modeling of the nitrogen co-metabolism in *Methylococcus capsulatus* (Bath)**. Biotechnology and Bioengineering, Vol. 116, No. 11, 2019, pp. 2884-2895.

Qian, Hongliang; Chen, Wei; Zhu, Weiwei; Liu, Chang; Lu, Xiaohua; Guo, Xiaojing; Huang, Dechun; Liang, Xiaodong; Kontogeorgis, Georgios M. / **Simulation and evaluation of utilization pathways of biomasses based on thermodynamic data prediction**. Energy, Vol. 173, 2019, pp. 610-625.

Ramirez-Castelan, Carlos E.; Hidalgo-Vivas, Angelica; Brix, Jacob; Jensen, Anker D.; Huusom, Jakob K. / **Mathematical Modelling and Simulation of a Trickle-Bed Reactor for Hydrotreating of Petroleum Feedstock**. International Journal of Chemical Reactor Engineering, Vol. 17, No. 7, 2019, pp. 1-27.

Rasmussen, Henrik; Wingstrand, Sara L.; Hassager, Ole / **On the universality in the extensional rheology of monodisperse polymer melts and oligomer dilutions thereof**. Rheologica Acta, Vol. 58, No. 6-7, 2019, pp. 333-340.

Raun, Kristian V.; Johannessen, Jeppe; McCormack, Kaylee; Appel, Charlotte C.; Baier, Sina; Thorhauge, Max; Høj, Martin; Jensen, Anker D. / **Modeling of the molybdenum loss in iron molybdate catalyst pellets for selective oxidation of methanol to formaldehyde**. Chemical Engineering Journal, Vol. 361, 2019, pp. 1285-1295.

Raun, Kristian V.; Thorhauge, Max; Høj, Martin; Jensen, Anker D. / **Modeling of molybdenum transport and pressure drop increase in fixed bed reactors used for selective oxidation of methanol to formaldehyde using iron molybdate catalysts**. Chemical Engineering Science, Vol. 202, 2019, pp. 347-356.

Ravenni, Giulia; Elhami, Omid H.; Ahrenfeldt, Jesper; Henriksen, Ulrik B.; Neubauer, York / **Adsorption and decomposition of tar model compounds over the surface of gasification char and active carbon within the temperature range 250-800°C**. Applied Energy, Vol. 241, 2019, pp. 139-151.

Ren, Tao; Modest, Michael F.; Fateev, Alexander; Sutton, Gavin; Zhao, Weijie; Rusu, Florin / **Machine learning applied to retrieval of temperature and concentration distributions from infrared emission measurements**. Applied Energy, Vol. 252, 2019, pp. 1-15.

Roager, Henrik M.; Vogt, Josef K.; Kristensen, Mette; Hansen, Lea B. S.; Ibrügger, Sabine; Mærkedahl, Rasmus B.; Bahl, Martin I.; Lind, Mads V.; Nielsen, Rikke L.; Frøkiær, Hanne; Gøbel, Rikke J.; Landberg, Rikard; Ross, Alastair B.; Brix, Susanne; Holck, Jesper; Meyer, Anne S.; Sparholt, Morten H.; Christensen, Anders F.; Carvalho, Vera; Holst, Jens J.; Rumessen, Jüri J.; Linneberg, Allan; Sicheritz-Pontén, Thomas; Dalgaard, Marlene D.; Blennow, Andreas; Frandsen, Henrik L; Villas-Bôas, Silas G; Kristiansen, Karsten; Vestergaard, Henrik; Hansen, Torben; Ekstrøm, Claus T.; Ritz, Christian; Nielsen, Henrik B.; Pedersen, Oluf B.; Gupta, Ramneek; Lauritzen, Lotte; Licht, Tine R. / **Whole grain-rich diet reduces body weight and systemic low-grade inflammation without inducing major changes of the gut microbiome: a randomised cross-over trial**. Gut, Vol. 68, No. 1, 2019, pp. 83-93.

Ruales-Salcedo, Angela V.; Higuita, Juan C.; Fontalvo, Javier; Woodley, John M. / **Design of enzymatic cascade processes for the production of low-priced chemicals**. Zeitschrift fuer Naturforschung. Section C: A Journal of Biosciences, Vol. 74, No. 3-4, 2019, pp. 77-84.

Salvinder, Kaur M. S.; Zabiri, Haslinda; Taqvi, Syed A.; Ramasamy, Marappa; Isa, Faezah; Rozali, Nor E. M.; Suleman, Humbul; Maulud, Abdulhalim; Shariff, Azmi M. / **An overview on control strategies for CO_2 capture using absorption/stripping system**. Chemical Engineering Research and Design, Vol. 147, 2019, pp. 319-337.

Sanahuja-Embuena, Victoria; Khensir, Gabriel; Yusuf, Mohamed; Andersen, Mads F.; Nguyen, Xuan T.; Trzaskus, Krzysztof; Pinelo, Manuel; Hélix-Nielsen, Claus / **Role of Operating Conditions in a Pilot Scale Investigation of Hollow Fiber Forward Osmosis Membrane Modules**. Membranes, Vol. 9, No. 6, 2019, pp. 1-28.

Sandoval, Diego R.; Michelsen, Michael L.; Yan, Wei; Stenby, Erling H. / **VT-Based Phase Envelope and Flash Calculations in the Presence of Capillary Pressure**. Industrial and Engineering Chemistry Research, Vol. 58, No. 13, 2019, pp. 5291-5300.

Sathish, Ashik; Sharma, Ashokkumar; Gable, Preston; Skiadas, Ioannis; Brown, Robert; Wen, Zhiyou / **A novel bulk-gas-to-atomized-liquid reactor for enhanced mass transfer efficiency and its application to syngas fermentation**. Chemical Engineering Journal, Vol. 370, 2019, pp. 60-70.

Schwarzer, Lars; Sárossy, Zsuzsa; Jensen, Peter A.; Glarborg, Peter; Karlström, Oskar; Holm, Jens K.; Dam-Johansen, Kim / **Kinetic Parameters for Biomass under Self-Ignition Conditions: Low-Temperature Oxidation and Pyrolysis**. Energy & Fuels, Vol. 33, No. 9, 2019, pp. 8606-8619.

Semenova, Daria; Silina, Yuliya E. / **The Role of Nanoanalytics in the Development of Organic-Inorganic Nanohybrids-Seeing Nanomaterials as They Are**. Nanomaterials, Vol. 9, No. 12, 2019, pp. 1-24.

Semenova, Daria; Silina, Yuliya E.; Koch, Marcus; Micheli, Laura; Zubov, Alexandr; Gernaey, Krist V. / **Sensors for biosensors: a novel tandem monitoring in a droplet towards efficient screening of robust design and optimal operating conditions**. Analyst, Vol. 144, No. 8, 2019, pp. 2511-2522.

Shahid, Muhammad Z.; Maulud, Abdulhalim S.; Bustam, Azmi M.; Suleman, Humbul; Halim, Hairul N. A.; Shariff, Azmi M. / **Rate-Based Modeling for Packed Absorption Column of the MEA-CO_2-Water System at High-Pressure and High-CO_2 Loading Conditions**. Industrial and Engineering Chemistry Research, Vol. 58, 2019, pp. 12235−12246.

Shen, Peng; Moghaddam, Saeed Z.; Huang, Qian; Daugaard, Anders E.; Zhang, Suojiang; Szabo, Peter / **Hard-soft thiol-ene materials without interfacial weakness**. Materials Today Communications, Vol. 21, 2019, pp. 1-7.

Shi, Meng; Lang, Xuemei; Wang, Yanhong; von Solms, Nicolas; Fan, Shuanshi / **Investigation of the Growth Kinetics of Tetra-n-butylammonium Bromide Hydrate Formation in Small Spaces**. Energy and Fuels, Vol. 33, No. 4, 2019, pp. 3473-3482.

Sigurdardóttir, Sigyn B.; Sueb, Mohd S. M.; Pinelo, Manuel / **Membrane compaction, internal fouling, and membrane preconditioning as major factors affecting performance of solvent resistant nanofiltration membranes in methanol solutions**. Separation and Purification Technology, Vol. 227, 2019, pp. 1-8.

Silina, Yuliya E.; Semenova, Daria; Spiridonov, Aleksey B. / **One-step encapsulation, storage and controlled release of low molecular weight organic compounds via electroplated nanoparticles**. The Analyst, Vol. 144, 2019, pp. 5677-5681.

Song, Ting; Deng, Jing; Deng, Liyuan; Bai, Lu; Zhang, Xiangping; Zhang, Suojiang; Szabo, Peter; Daugaard, Anders E. / **Poly(vinylimidazole-co-butyl acrylate) membranes for CO_2 separation**. Polymer, Vol. 160, 2019, pp. 223-230.

Spann, Robert; Gernaey, Krist V.; Sin, Gürkan / **A compartment model for risk-based monitoring of lactic acid bacteria cultivations**. Biochemical Engineering Journal, Vol. 151, 2019, pp. 1-11.

Spann, Robert; Glibstrup, Jens; Pellicer-Alborch, Klaus; Junne, Stefan; Neubauer, Peter; Roca, Christophe; Kold, David; Lantz, Anna E.; Sin, Gürkan; Gernaey, Krist V.; Krühne, Ulrich / **CFD predicted pH gradients in lactic acid bacteria cultivations**. Biotechnology and Bioengineering, Vol. 116, No. 4, 2019, pp. 769-780.

Stummann, Magnus Z.; Hansen, Asger B.; Hansen, Lars P.; Davidsen, Bente; Rasmussen, Søren B.; Wiwel, Peter; Gabrielsen, Jostein; Jensen, Peter A.; Jensen, Anker D.; Høj, Martin / **Catalytic Hydropyrolysis of Biomass using Molybdenum Sulfide Based Catalyst. Effect of Promoters**. Energy and Fuels, Vol. 33, No. 2, 2019, pp. 1302-1313.

Stummann, Magnus Z.; Høj, Martin; Davidsen, Bente; Hansen, Lars P.; Beato, Pablo; Gabrielsen, Jostein; Jensen, Peter A.; Jensen, Anker D. / **Deactivation of a CoMo catalyst during catalytic hydropyrolysis of biomass. Part II: Characterization of the spent catalysts and char**. Energy and Fuels, Vol. 33, No. 12, 2019, pp. 12387-12402.

Stummann, Magnus Z.; Høj, Martin; Hansen, Asger B.; Beato, Pablo; Wiwel, Peter; Gabrielsen, Jostein; Jensen, Peter A.; Jensen, Anker D. / **Deactivation of a CoMo catalyst during catalytic hydropyrolysis of biomass. Part I: Product distribution and composition**. Energy and Fuels, Vol. 33, No. 12, 2019, pp. 12374-12386.

Stummann, Magnus Z.; Høj, Martin; Hansen, Asger B.; Davidsen, Bente; Wiwel, Peter; Gabrielsen, Jostein; Jensen, Peter A.; Jensen, Anker D. / **New insights into the effect of pressure on catalytic hydropyrolysis of biomass**. Fuel Processing Technology, Vol. 193, 2019, pp. 392-403.

Su, Jun; Li, Caihong / **Combined effect of modified titanium carbide (TiC) particles and ethylene alpha olefins (POE) on properties of ethylene propylene diene monomer (EPDM)/TiC/POE composites for electronic application**. Journal of Materials Science: Materials in Electronics, Vol. 30, No. 4, 2019, pp. 4164-4173.

Su, Jun; Zhang, Jun / **Recent development on modification of synthesized barium titanate ($BaTiO_3$) and polymer/$BaTiO_3$ dielectric composites**. Journal of Materials Science: Materials in Electronics, Vol. 30, No. 3, 2019, pp. 1957-1975.

Sun, Li; Kontogeorgis, Georgios M.; von Solms, Nicolas; Liang, Xiaodong / **Modeling of Gas Solubility Using the Electrolyte Cubic Plus Association Equation of State**. Industrial and Engineering Chemistry Research, Vol. 58, No. 37, 2019, pp. 17555-17567.

Sun, Li; Liang, Xiaodong; Solms, Nicolas von; Kontogeorgis, Georgios M. / **Modeling Tetra-n-butyl ammonium halides aqueous solutions with the electrolyte cubic plus association equation of state**. Fluid Phase Equilibria, Vol. 486, 2019, pp. 37-47.

Sutton, Gavin; Fateev, Alexander; Rodríguez-Conejo, Miguel A.; Meléndez, Juan; Guarnizo, Guillermo / **Validation of Emission Spectroscopy Gas Temperature Measurements Using a Standard Flame Traceable to the International Temperature Scale of 1990 (ITS-90)**. International Journal of Thermophysics, Vol. 40, No. 99, 2019, pp. 1-36.

Syalsabila, Afaf; Maulud, Abdulhalim S.; Suleman, Humbul; Hadi Md Nordin, Nik A. / **Corrigendum to "VLE of Carbon Dioxide-Loaded Aqueous Potassium Salt of L-Histidine Solutions as a Green Solvent for Carbon Dioxide Capture: Experimental Data and Modelling"**. International Journal of Chemical Reactor Engineering, Vol. 2019, 2019, pp. 1-2.

Syalsabila, Afaf; Maulud, Abdulhalim S.; Suleman, Humbul; Hadi Md Nordin, Nik A. / **VLE of Carbon Dioxide-Loaded Aqueous Potassium Salt of L -Histidine Solutions as a Green Solvent for Carbon Dioxide Capture: Experimental Data and Modelling**. International Journal of Chemical Reactor Engineering, Vol. 2019, 2019, pp. 1-12.

Tajsoleiman, Tannaz; Mears, Lisa; Krühne, Ulrich; Gernaey, Krist V.; Cornelissen, Sjef / **An Industrial Perspective on Scale-Down Challenges Using Miniaturized Bioreactors**. Trends in Biotechnology, Vol. 37, No. 7, 2019, pp. 697-706.

Tajsoleiman, Tannaz; Spann, Robert; Bach, Christian; Gernaey, Krist V.; Huusom, Jakob K.; Krühne, Ulrich / **A CFD based automatic method for compartment model development**. Computers and Chemical Engineering, Vol. 123, 2019, pp. 236-245.

Tong, Jiahuan; Xiao, Xingqing; Liang, Xiaodong; von Solms, Nicolas; Huo, Feng; He, Hongyan; Zhang, Suojiang / **Insights into the solvation and dynamic behaviors of a lithium salt in organic- and ionic liquid-based electrolytes**. Physical Chemistry Chemical Physics, Vol. 21, 2019, pp. 19216-19225.

Trifol, Jon; van Drongelen, Martin; Clegg, Francis; Plackett, David; Szabo, Peter; Daugaard, Anders E. / **Impact of thermal processing or solvent casting upon crystallization of PLA nanocellulose and/or nanoclay composites**. Journal of Applied Polymer Science, Vol. 136, No. 20, 2019, pp. 1-14.

Ullah, Sami; Suleman, Humbul; Tahir, Muhammad S.; Sagir, Muhammad; Muhammad, Shabbir; Al-Sehemi, Abdullah G.; Zafar, Masood-ur-Rauf; Kareem, Firas A. A.; Maulud, Abdulhalim S.; Bustam, Mohamad A. / **Reactive kinetics of carbon dioxide loaded aqueous blend of 2-amino-2-ethyl-1,3-propanediol and piperazine using a pressure drop method**. International Journal of Chemical Kinetics, Vol. 51, No. 4, 2019, pp. 291-298.

Ulusoy, Burak; Lin, Weigang; Karlström, Oskar; Li, Songgeng; Song, Wenli; Glarborg, Peter; Dam-Johansen, Kim; Wu, Hao / **Formation of NO and N_2O during Raw and Demineralized Biomass Char Combustion**. Energy and Fuels, Vol. 33, No. 6, 2019, pp. 5304-5315.

Ulusoy, Burak; Wu, Hao; Lin, Weigang; Karlström, Oskar; Li, Songgeng; Song, Wenli; Glarborg, Peter; Dam-Johansen, Kim / **Reactivity of sewage sludge, RDF, and straw chars towards NO**. Fuel, Vol. 236, 2019, pp. 297-305.

Vaicekauskaite, Justina; Yang, Canhui; Skov, Anne L.; Suo, Zhigang / **Electric field concentration in hydrogel-elastomer devices**. Extreme Mechanics Letters, Vol. 34, 2019, pp. 1-6.

Vaicekauskaite, Justina; Mazurek, Piotr; Vudayagiri, Sindhu; Skov, Anne L. / **Mapping the mechanical and electrical properties of commercial silicone elastomer formulations for stretchable transducers**. Journal of Materials Chemistry C, Vol. 8, 2019, pp. 1273-1279.

Villadsen, Sebastian N. B.; Fosbøl, Philip L.; Angelidaki, Irini; Woodley, John M.; Nielsen, Lars P.; Møller, Per / **The Potential of Biogas; The Solution to Energy Storage**. ChemSusChem, Vol. 12, No. 10, 2019, pp. 2147-2153.

Wang, Guoliang; Jensen, Peter A.; Wu, Hao; Frandsen, Flemming J.; Laxminarayan, Yashasvi; Sander, Bo; Glarborg, Peter / **KOH capture by coal fly ash**. Fuel, Vol. 242, 2019, pp. 828-836.

Wang, Guoliang; Jensen, Peter A.; Wu, Hao; Frandsen, Flemming J.; Laxminarayan, Yashasvi; Sander, Bo; Glarborg, Peter / **Potassium capture by coal fly ash K_2CO_3, KCl and K_2SO_4**. Fuel Processing Technology, Vol. 194, 2019, pp. 1-11.

Wang, Tianyuan; Guittard, Philippe; Coquelet, Christophe; El Ahmar, Elise; Baudouin, Olivier; Kontogeorgis, Georgios M. / **Corrigendum to "Improvement of the PR-CPA equation of state for modelling of acid gases solubilities in aqueous alkanolamine solutions" [Fluid Phase Equilibria, vol. 471, 2018, 74-87]**. Fluid Phase Equilibria, Vol. 485, 2019, pp. 126-127.

Wang, Wendi; Madsen, Peter; Skov, Anne L.; Huang, Qian / **Improvement of mechanical properties of anisotropic glassy polystyrene by introducing heatlabile reversible bonds**. Macromolecules, Vol. 52, No. 23, 2019, pp. 9261-9271.

Wang, Xueting; Huang, Yixin; Erik Weinell, Claus; Olsen, Stefan M.; Kiil, Søren / **Leveling kinetics of coatings with solvent evaporation and non-Newtonian rheology**. Progress in Organic Coatings, Vol. 132, 2019, pp. 169-177.

Wang, Xueting; Erik Weinell, Claus ; Tobar, Vicenç; Olsen, Stefan M.; Kiil, Søren / **Leveling measurements of antifouling coatings using an optical profilometer: Effects of additives and solvent concentration and type**. Progress in Organic Coatings, Vol. 132, 2019, pp. 159-168.

Wang, Zhen; Chen, Xue-Ming; Ni, Bing Jie; Tang, You N.; Zhao, He-Ping / **Model-based assessment of chromate reduction and nitrate effect in a methane-based membrane biofilm reactor**. Water Research X, Vol. 5, 2019, pp. 1-8.

Woodley, John M. / **Accelerating the implementation of biocatalysis in industry**. Applied Microbiology and Biotechnology, Vol. 103, No. 12, 2019, pp. 4733–4739.

Woodley, John M. / **New Frontiers in Biocatalysis for Sustainable Synthesis**. Current Opinion in Green and Sustainable Chemistry, Vol. 21, 2019, pp. 22-26.

Woodley, John M. / **Reaction Engineering for the Industrial Implementation of Biocatalysis**. Topics in catalysis, Vol. 62, No. 17-20, 2019, pp. 1202-1207.

Yang, Jifeng; Bhagat, Rajesh K.; Fernandes, Rubens R.; Nordkvist, Mikkel; Gernaey, Krist V.; Krühne, Ulrich; Wilson, D. Ian / **Cleaning of toothpaste from vessel walls by impinging liquid jets and their falling films: Quantitative modelling of soaking effects**. Chemical Engineering Science, Vol. 208, pp. 1-15.

Yang, Jifeng; Kjellberg, Kim; Jensen, Bo B. B.; Nordkvist, Mikkel; Gernaey, Krist V.; Krühne, Ulrich / **Investigation of the cleaning of egg yolk deposits from tank surfaces using continuous and pulsed flows**. Food and Bioproducts Processing, Vol. 113, 2019, pp. 154-167.

Zdarta, Jakub; Bachosz, Karolina; Degórska, Oliwia; Zdarta, Agata; Kaczorek, Ewa; Pinelo, Manuel; Meyer, Anne S.; Jesionowski, Teofil / **Co-Immobilization of Glucose Dehydrogenase and Xylose Dehydrogenase as a New Approach for Simultaneous Production of Gluconic and Xylonic Acid**. Materials, Vol. 12, No. 19, 2019, pp. 1-16.

Zdarta, Jakub; Meyer, Anne S.; Jesionowski, Teofil; Pinelo, Manuel / **Multi-faceted strategy based on enzyme immobilization with reactant adsorption and membrane technology for biocatalytic removal of pollutants: A critical review**. Biotechnology Advances, Vol. 37, No. 7, 2019, pp. 1-21.

Zdarta, Jakub; Jankowska, Katarzyna; Wyszowska, Marta; Kijeńska-Gawrońska, Ewa; Zgoła-Grześkowiak, Agnieszka; Pinelo, Manuel; Meyer, Anne S.; Moszyński, Dariusz; Jesionowski, Teofil / **Robust biodegradation of naproxen and diclofenac by laccase immobilized using electrospun nanofibers with enhanced stability and reusability**. Materials Science and Engineering C: Biomimetic Materials, Sensors and Systems, Vol. 103, 2019, pp. 1-10.

Zeng, Ying; Erik Weinell, Claus; Dam-Johansen, Kim; Ring, Louise; Kiil, Søren / **Exposure of hydrocarbon intumescent coatings to the UL1709 heating curve and furnace rheology: Effects of zinc borate on char properties**. Progress in Organic Coatings, Vol. 135, 2019, pp. 321-330.

Zhang, Wei; Liu, Jizhen; Gao, Mingming; Pan, Chenyang; Huusom, Jakob K. / **A fault early warning method for auxiliary equipment based on multivariate state estimation technique and sliding window similarity**. Computers in Industry, Vol. 107, 2019, pp. 67-80.

Zhang, Wei; Liu, Jizhen; Gao, Ming-ming; Huusom, Jakob K. / **A novel operation cost optimization system for mix-burning coal slime circulating fluidized bed boiler unit**. Applied Thermal Engineering, Vol. 148, 2019, pp. 620-631.

Zhang, Hao; Luo, Jianquan; Li, Sushuang; Woodley, John M.; Wan, Yinhua / **Can graphene oxide improve the performance of biocatalytic membrane?**. Chemical Engineering Journal, Vol. 359, 2019, pp. 982-993.

Contributions to books and reports

Eslahpazir, Manely; Krull, Rainer; Krühne, Ulrich / **Computational Fluid Dynamics**. Comprehensive Biotechnology. Editor / M. Moo-Young. Vol. 2 3.ed. Elsevier, 2019. pp. 95-107.

Jensen, Peter A.; Laxminarayan, Yashasvi; Wang, Guoliang; Schwarzer, Lars; Sander, Bo; Holm, Jens K.; Frandsen, Flemming; Wu, Hao; Glarborg, Peter; Wedel, Stig; Dam-Johansen, Kim / **Final report: Flexible use of biomass on PF Fired power plants**. 2019.

Li, Xiaoxi; Rubæk, Gitte H.; Müller-Stöver, Dorette S.; Thomsen, Tobias P.; Ahrenfeldt, Jesper; Sørensen, Peter / **Plant Availability of Phosphorus in Five Gasification Biochars**. New Processes for Nutrient Recovery from Wastes. Editor / Matias B. Vanotti; Maria C. García-González; Beatriz Molinuevo-Salces; Berta Riaño. Frontiers Media S.A., 2019. pp. 62-73 (Frontiers Research Topics).

Mansouri, Seyed S.; Gargalo, Carina L.; Udugama, Isuru A.; Ramin, Pedram; Sales-Cruz, Mauricio; Sin, Gürkan; Gernaey, Krist V. / **Economic Risk Analysis and Critical Comparison of Biodiesel Production Systems**. Biodiesel. From Production to Combustion. Editor / Meisam Tabatabaei; Mortaza Aghbashlo. Springer, 2019. pp. 127-148 (Biofuel and Biorefinery Technologies, Vol. 8).

Mikkelsen, Peter S.; Arnbjerg-Nielsen, Karsten; Bjerg, Poul L.; Bauer-Gottwein, Peter; Albrechtsen, Hans-Jørgen; Andersen, Henrik R.; Vezzaro, Luca; Borup, Morten; Hansen, Lisbeth T.; Drews, Martin; Mølhave, Kristian; Gernaey, Krist V.; Stedmon, Colin; Mariani, Patrizio; Ramousse, Severine; Jensen, Lotte B.; Madsen, Henrik; Christiansen, Lasse E.; Christensen, Erik D.; Jepsen, Peter U.; Janting, Jakob; Ruepp, Sarah R.; Pedersen, Christian; Poulsen, Line B.; Overgaard Jensen, Thomas; Brückner, Lars; Molzen, Jan E.; Andersen, Morten; Odgaard, Mads H. / **Lad vand og data strømme**. Kgs. Lyngby : Danmarks Tekniske Universitet (DTU), 2019. pp. 1-71.

Nazemzadeh, Nima; A. Udugama, Isuru; Fjordbak Nielsen, Rasmus; Meyer, Kristian; Perez-Cisneros, Eduardo S.; Sales-Cruz, Mauricio; Huusom, Jakob K.; Abildskov, Jens; Mansouri, Seyed S. / **Graphical tools for designing intensified distillation processes: Methods and applications**. Process Intensification: Design Methodologies. Editor / Fernando Israel Gómez-Castro; Juan Gabriel Segovia-Hernández. De Gruyter, 2019. pp. 145-179.

Nazemzadeh, Nima; Udugama, Isuru A.; Taube, Michael A.; Abildskov, Jens; Mansouri, Seyed S. / **Molecular tracking: A novel approach for multicomponent distillation column design**. Computer Aided Chemical Engineering. Editor / Anton A. Kiss; Edwin Zondervan; Richard Lakerveld; Leyla Özkan. Elsevier, 2019. pp. 313-318 (Computer Aided Chemical Engineering, Vol. 46).

Plósz, Benedek Gy.; Ramin, Pedram / **Wastewater-Based Epidemiological Engineering—Modeling Illicit Drug Biomarker Fate in Sewer Systems as a Means To Back-Calculate Urban Chemical Consumption Rates**. Wastewater-Based Epidemiology: Estimation of Community Consumption of Drugs and Diets. Editor / Bikram Subedi; Daniel A. Burgard; Bommanna G. Loganathan. American Chemical Society, 2019. pp. 99-115 (A C S Symposium Series, Vol. 1319).

Puig-Arnavat, Maria; Thomsen, Tobias P.; Ravenni, Giulia; Clausen, Lasse R.; Sárossy, Zsuzsa; Ahrenfeldt, Jesper / **Pyrolysis and Gasification of Lignocellulosic Biomass**. Biorefinery: Integrated Sustainable Processes for Biomass Conversion to Biomaterials, Biofuels, and Fertilizers. Editor / Juan-Rodrigo Bastidas-Oyanedel; Jens Ejbye Schmidt. Cham: Springer, 2019. pp. 79-110.

PhD thesis defences **2019**

Adam Karcz
Surface characterization of activated chalcopyrite particles

Anders Schlaikjer
Development of the electrolyte CPA Equation of State

Anna Leth-Espensen
Modeling bio-dust combustion in suspension firing

Antonio Grimalt Alemany
Syngas fermentation to biofuels: Evaluation of the interplay of kinetics and thermodynamics for directing bioconversions based on mixed microbial communities

Burak Ulusoy
NO_x formation and reduction in fluidized bed combustion of biomass

Carlos Eduardo Ramírez Castelán
Mathematical modelling and simulation of a trickle-bed reactor for petroleum feedstocks hydrotreatin

Chitta Ranjan Behera
A decision support tool for screening novel WWT processes

Francois Kruger
Towards the realization of subsea factories: Thermodynamics of petroleum fluids relevant to subsea processing

Frederico C.C. Montes
In-silico process design and evaluation tool for pharmaceutical manufacturing

Giulia Ravenni
Application of biomass char to tar conversion and producer gas upgrading to syngas

Hao Luo
Modelling of biomass combustion and gasification: From particle-scale to reactor-scale

Héctor Alexánder Forero-Hernández
Validation and improvement of property and process modeling for oleochemicals

Jifeng Yang
Novel strategies for cleaning-in-place operations

Kasper Hartvig Lejre
Mechanisms of sulfur dioxide and sulfuric acid neutralization in lube oil for marine diesel engines

Katrin Pontius
Monitoring of bioprocesses. Opportunities and challenges

Konstantinos Asimakopoulos
Biomethanation of synthesis gas in trickle bed reactors

Kristian Meyer
Advanced simulation of preparative chromatography processes

Lars Schwarzer
Biomass particle ignition in mill equipment

Li Sun
Analysis and applications of the e-CPA Equation of State

Lukasz Ruszczynski
Thermodynamic modelling and data evaluation for life sciences applications

Magnus Zingler Stummann
Catalytic hydropyrolysis for green fuels

Mark Nicholas Jones
Design and optimisation of oleochemical processes

Marvin Masche
Milling and physical properties of wood pellets for suspension-fired power plan

Nipun Garg
Phenomena-based process synthesis-intensification

Peter S. Hammershøi
Durable zeolite based catalyst systems for diesel emission control

Ricardo André Fernandes Caroço
Model-based monitoring and optimization of a bio-based process

Robert Timo Hagemann
Causes and consequences of Aspergillus niger pelleting behaviour in industrial cultivation

Spardha Virendra Jhamb
Computer-aided design of sustainable product formulations

Ying Zeng
Performance studies and char characterizations of hydrocarbon intumescent coatings

Ting Song
Membrane modification, preparation and application

Yu Zhang
Catalytic oxidation of methane

Xianglei Meng
Conversion of CO_2 to carbonates catalyzed by ionic liquids under mild conditions

Zhibo Zhang
Use of ionic liquids and support materials for high performance - enzymatic conversion of CO_2 into formic acid and formaldehyde

Publisher
Department of Chemical and Biochemical Engineering
Building 228A
2800 Kgs. Lyngby
Denmark
Phone +45 4525 2822
Email kt@kt.dtu.dk
Web www.kt.dtu.dk

Annual Report 2019
June 2020
ISBN: 978-87-3054-89-9

Editor in chief
Professor Kim Dam-Johansen, Head of Department

Executive editor
Lonnie Jørgensen, Communications Officer

Articles
Morten Andersen, Journalist

Editorial support
Frederik Appel Olsen, Communications Officer
Meile Adinaviciute, Student worker

Photos
Anne Birgitte Skovholm Hedegaard
Ying Zeng
Christian Ove Carlsson
Thorkild Christensen
Outreach-now

Cover photo
Christian Ove Carlsson

Design and print
STEP PRINT POWER

FSC www.fsc.org MIX Paper from responsible sources FSC® C011323

Nordic Swan Ecolabel Printed matter 5041 0072

This Annual Report 2019 may be ordered from the reception at the Department of Chemical and Biochemical Engineering, DTU

Phone +45 4525 2822
Email kt@kt.dtu.dk

Also available on www.kt.dtu.dk

Follow DTU Chemical Engineering on

LinkedIn

www.linkedin.com/company/398282