Technical University of Denmark

# Annual Report **2017**

**DTU Chemical Engineering**
Department of Chemical and Biochemical Engineering

# Key numbers for 2017

The vision of DTU Chemical Engineering is to be acknowledged as a world-leading chemical and biochemical-engineering department. Below we have listed a selection of our key results in 2017 to show how they support our strategic objectives.

| STRATEGIC AREA | VISION | RESULTS IN 2017 |
|---|---|---|
| RESEARCH | Supports the development of sustainable solutions in the fields of chemistry, biotechnology, food, pharma, and energy through research and scientific advice. | **210** SCIENTIFIC ARTICLES IN WOS-INDEXED JOURNALS<br>**1** BOOKS & MONOGRAPHS<br>**6** CONTRIBUTIONS TO BOOKS<br>**31** PHD THESES DEFENCES |
| INNOVATION | An attractive partner for university departments and research-based industry. | **11** INDUSTRIAL PHDS<br>**2** INDUSTRIAL POSTDOC<br>In cooperation with Coloplast, Novozymes, Hempel, Haldor Topsøe, DuPont, Novo Nordisk, Freesense, Unibio, Rockwool International, Grundfos, and PHX Innovation |
| EDUCATION | Helps to retain, develop, and attract knowledge-based national working places, including companies with affiliates abroad. | **319** STUDENTS (STÅ*)<br>**22,6** SINO-DANISH STUDENTS (STÅ*)<br>**37** COMPLETED BENG PROJECTS<br>**25** COMPLETED BSC PROJECTS<br>**70** COMPLETED MSC PROJECTS |
| ORGANIZATION | Attractive place to work for ambitious and technology-passionate staff members. | **52** TECHNICAL/ADMINISTRATIVE EMPLOYEES (FTE**)<br>**111** PHD STUDENTS (FTE**)<br>**99** SCIENTIFIC EMPLOYEES (FTE**)<br>**262** EMPLOYEES IN TOTAL (FTE**)<br>**33** FACULTY MEMBERS |

| STAFF DISTRIBUTED BY AGE: | INTERNATIONAL SCIENTIFIC STAFF: |
|---|---|
| **37%** 20-29 | **4%** AFRICA |
| **34%** 30-39 | **30%** ASIA |
| **11%** 40-49 | **58%** EUROPE |
| **11%** 50-59 | **5%** MIDDLE EAST |
| **6%** 60-69 | **1%** NORTH AMERICA |
| **1%** 70-80 | **2%** SOUTH AMERICA |

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

Front page photo:
Ming Liu and Caroline Mosbech working in the BioEng lab, where tailored enzymes are applied for optimized biomass conversion and synthesis of bioactive compounds. Photo: Thorkild Christensen

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A tailor-made rotor setup used for the characterization and testing of non-fouling coatings in the PhD research study by Xueting Wang at DTU Chemical Engineering CoaST Research Centre.

Photo: Thorkild Christensen

# Welcome

Welcome to our Annual Report 2017. This year has been a year of growth, new collaborations, and remarkable results.

## Education to the benefit of the industry

Education and research is at the heart of our department. We offer a wide range of educational programmes, all with their basis in the core disciplines of chemical engineering. In 2017, we led 83 courses at Bachelor's and Master's level, 11 of which within the frames of the Sino-Danish Center for Education and Research. We also facilitated a large experimental summer course for 66 American students and 15 Chinese students at our annual Summer University and taught 11 PhD or combined PhD and continuing education courses. Our faculty has been busy providing our students with the best education possible—to the benefit of both domestic and international industry in the field.

## Strong research and innovation

Our education is research-based and therefore dependent on strong research environments at the department, covering the important areas of chemical and biochemical engineering. The landscape is constantly changing, and we are continuously seeking to adapt our research themes according to present and future needs and funding opportunities. In this way, we have secured a large degree of stability and development over the years. In 2017, we have also seen a considerable development with many new projects and collaborations and raised significant funding that will secure a strong future development within biotechnological production in collaboration with other DTU departments—and within coatings science and technology within the frames of the new Hempel Foundation Coatings Science and Technology Centre.

A large part of our research and innovation happens in the form of PhD projects. 31 PhD students have finished their projects during 2017, and we have taken in a corresponding number of new PhD students. This large amount of activity creates a dynamic setting where new areas are gradually implemented as new needs and funding arise. One of the remarkable results in 2017 was when Associate Professor Anne Ladegaard Skov defended her doctoral thesis and received the degree of Doctor Technices at the annual DTU Commemoration Day.

## Close collaborations with industry

Many of our activities are carried out in close collaboration with industry, an important part of our field of operation. Examples of this are seen within BIOPRO under the leadership of Professor Krist V. Gernaey, and the consolidation of our KT Consortium, where we collaborate with large international companies within process systems engineering. We expect development within this area in order to cover an increasing amount of activities at our department in the years to come. During 2017, Professor Georgios Kontogeorgis took over the leadership of KT Consortium from Professor Rafiqul Gani who retired at the end of the year after a very productive career. I want to thank Professor Gani for his great contribution to the development of the department. I also would like to thank Lars G. Kiørboe for many years as head of our Pilot Plant, a position taken over by Steen Larsen. We welcome Steen with great expectations for the future development of the Pilot Plant.

As mentioned above, our department is experiencing a very positive development with still more students and expanding research activity. More activity inevitably leads to an increased pressure on our infrastructure. Luckily, this year we have initiated the design of our new Building 228A with expected completion by January 2020. The new facilities will contain both laboratories and pilot halls. This extensive project will demand a significant effort in the next couple of years.

It is a privilege to be heading an organization with so many talented and dedicated employees in all positions, and with a constant inflow of new, energetic students. The future looks promising. I hope that you will enjoy reading about our great many activities as you flip through the pages of this annual report for 2017.

Kim Dam-Johansen
*Professor, Head of Department*


# HIGHLIGHTS

**GREEN CHALLENGE**
SDC students sharing their green projects at the 2017 Grøn Dyst (Green Challenge) at DTU. The Green Challenge is a student conference where future engineers meet, share, and inspire each other within environmental sustainability.


Photo: Niels Grolin ①


②


Photo: Thorkild Christensen ③


④


Photo: Sanne Vils Unge Forskere ⑤


Photo: Tom Jersø/ATV ⑥

# HIGHLIGHTS **2017**

## JANUARY

**1 January**

### ESTABLISHMENT OF NEW RESEARCH CENTRE

As per 1 January 2017, the Hempel Foundation Coatings Science and Technology Centre (CoaST) was established. The centre, headed by Kim Dam-Johansen, will support development, production and use of coatings with improved sustainability profiles over the lifetime of the coating.

## FEBRUARY

**February**

### ANOTHER AWARD FOR MICROFLUIDICS VIDEOS

The video about Microfluidics won yet another award, this time as Best Animation Video at the Copenhagen Film Festival.

**20 February**

### METTE FREDERIKSEN VISITS DTU CHEMICAL ENGINEERING ①

Under the theme 'Creation and retention of industrial jobs in Denmark', the leader of the Social Democratic Party visited DTU Lyngby campus. Among many exciting activities on her schedule was a visit to our Pilot Plant where Head of Department Kim Dam-Johansen explained about some of our research.

## MARCH

**March**

### AN EXCURSION WITH POLYTECHNIC STUDENTS IN 1913 ②

In an essay written by Professor Emeritus John Villadsen, the very origins of chemical engineering in Denmark, and thus of our department as we know it today, are carefully described. The narrative takes its point of departure in an old photograph of a handful of young Danish polytechnic students visiting the Drägerwerk factory in Germany.

**17 March**

### ANNE LADEGAARD SKOV DEFENDED HER DR. TECH THESIS ③

Anne Ladegaard Skov defended her Dr. Tech thesis, five years' worth of research on 'Silicone-based Dielectric Elastomers'. Anne Ladegaard Skov's thesis provides the most thorough insight into the potential of dielectric elastomers to date within this scientific area. On 28 April, she received her degree at the annual DTU Commemoration Day.

**24 March**

### STATOIL PRIZE FOR RESEARCH INTO ARTIFICIAL MUSCLES

Associate Professor Anne Ladegaard Skov received the Statoil Award 2017 for her internationally acclaimed research within the field of dielectric elastomers.

## APRIL

**3 April**

### HEMPEL-DTU AWARD WINNERS ④ ⑤

Thirty students from Espergærde High School visited DTU for a day of science in connection with winning the 2016 Hempel-DTU Award for their efforts to engage students in engineering and science. Some of the many exciting experiences on the agenda were the marvellous world of paint science by Associate Professor Søren Kiil, a tour of the department's pilot facilities by Head of Pilot Plant Lars Kiørboe, and a tour of the Centre for Oil and Gas. The 2017 award was given to Holstebro Technical High School and Egaa High School by Head of Department Kim Dam-Johansen during the Unge Forskere (Young Scientist) competition in Copenhagen.

**26 April**

### ELASTYRENPRISEN TO OLE HASSAGER ⑥

The Danish polymer award ATV Elastyrenprisen was this year awarded to Professor Ole Hassager. The award was given in recognition of his long-standing career as researcher and educator within polymers and plastic where he has delivered research at a high level and is known to be an excellent teacher. In the motivation for the awarding of the prize, Ole Hassager's contributions within rheology—the study of fluidic and deformation properties of materials affected by mechanical forces—was emphasized.

## MAY

**5 May**

### COUNTRY SEMINAR IN PROSYS

The Process and Systems Engineering Centre (PROSYS) hosts a country seminar every year. During this seminar, new employees have a chance to introduce different aspects of their native countries: history, culture, and must-see places. The event ends up with tasting a variety of typical dishes from different counties, in a friendly atmosphere. This year, the seminar included presentations from Turkey, Poland, Portugal, Denmark, Czech Republic, Iran, Spain, India, and Colombia.

## JUNE

**6-8 June**

### KT CONSORTIUM ANNUAL MEETING AND ANNOUNCEMENT OF NEW HEAD OF KT CONSORTIUM ⑦

54 delegates from industry and academia from around the world were gathered for a three-day Annual Meeting in Elsinore north of Copenhagen. The focus of the conference was on how to ensure that research and innovation go hand in hand with the future needs of society. At the meeting, it was announced that Professor Georgios Kontogeorgis had been appointed new Head of KT Consortium. He succeeded Professor Rafiqul Gani, who for many years was Head of the CAPEC centre. Thanks to Professor Kontogeorgis' many years as Head of AT CERE, he is an experienced networker who has succeeded in building a large and strong consortium.

**21-23 June**

### CERE DISCUSSION MEETING

No less than 17 companies from 10 different countries were present at the 2017 CERE Discussion Meeting, reflecting on the strength of the CERE industrial Consortium.

**23 June**

### STRONGER DANISH-CHINESE COLLABORATION ⑧

A stronger collaboration was on the agenda as delegates from the Institute of Process Engineering, Chinese Academy of Sciences, and DTU Chemical Engineering met to discuss the aim of a joint research and education centre within Chemical and Biochemical Engineering under the existing Sino-Danish Center for Education and Research, also known as SDC. The completion of the seminar also provided a chance to see how 'green technologies' are being implemented in the programme in real life—as part of the Green Challenge at DTU. Both Danish and Chinese SDC students shared their green projects as part of the MSc programme. This year's Grøn Dyst (Green Challenge) student projects included: 'A green approach of production of aerogels from waste clothes', 'Sustainable production of algae at Avedøre—A case study', 'A membrane technology-based fresh-keeping device for fruit and vegetables', and 'Utilization of wastewater generated from sweet potato starch production for cultivation of functional strains'.


Photo: Christian Ove Carlsson ⑦


⑧


⑨


Photo: Bo Yan ⑩


Photo: Christian Ove Carlsson ⑪


Photo: Christian Ove Carlsson ⑫

# HIGHLIGHTS **2017**

## JULY

**2-6 July**

### DPC HOSTS ISPO CONFERENCE

The International Workshop on Silicone Polymers (ISP02017) was successfully held by the Danish Polymer Center (DPC). The conference comprised 96 participants from all over the world, representing 26 companies and 15 universities. Thirty-three presentations on silicone polymers were given, ranging from how to make science into innovations over advanced chemistries to characterization and utilization of silicone polymers and cross-linked silicone rubbers.

**3-28 July**

### SUMMER UNIVERSITY ⑨

Again this year, our Summer University brought together international students as no less than 66 students from the USA, two students from Italy, 15 students from the Sino-Danish Center (SDC), and four Danish DTU students worked hard in the Pilot Plant at DTU Chemical Engineering.

## AUGUST

**22 August**

### BIOENG ANNUAL RESEARCH DAY

BioEng celebrated their annual Research Day at Comwell Borupgaard. Everyone presented their projects and synergies and interdisciplinary collaboration were identified.

## SEPTEMBER

**22 September**

### PROFESSOR KIM DAM-JOHANSEN GAVE AN INVITED LECTURE AT TSINGHUA CHEMICAL ENGINEERING

Professor and Head of Department Kim Dam-Johansen gave an invited lecture at Tsinghua Chemical Engineering, China entitled 'Clean Energy and Quantitative Product Engineering—A history of research for the benefit of society'.

**24-25 September**

### NEW JOINT EDUCATION BASED RESEARCH AND INNOVATION CENTRE ⑩

After participating in the SDC workshop and the opening ceremony of the House of Danish Industry Foundation (DIF) SDC building with the presence of HRH Crown Prince Frederik, Head of Department Kim Dam-Johansen and Suojiang Zhang, Director of IPE, Chinese Academy of Sciences, signed the Memorandum of Understanding to establish the new joint Center for Sustainable Process Engineering. The centre is the result of many years of strong Danish-Chinese collaboration between the two partners.

## OCTOBER

**1-5 October**

### WORLD CONGRESS OF CHEMICAL ENGINEERING (WCCE10)

The WCCE conference series covers all aspects of chemical engineering, and was this year organized jointly with ESCAPE27, an annual event for everybody involved in process systems engineering. PROSYS participated with a delegation of 19 persons (faculty, postdocs, PhD students) to present the most prominent recent research results of PROSYS.

**9-11 October**

### NORDIC FLAME DAYS IN STOCKHOLM

The 2017 Nordic Flame Days is an annual event for everybody involved in combustion or combustion-related processes. CHEC participated with nine PhD students who presented their work.

**5-10 October**

### INSTALLATION OF THE YSTRAL, CONTI-TDS 1

CoaST established an industrial collaboration with Ystral Gmbh and Hempel A/S on in-line dispersion and wetting techniques in coating production. As part of the collaboration, an Ystral in-line mixer, Conti-TDS1, has been installed at the department.

**12 October**

### SCIENCE TALENT FORSKER CAMP VISIT ⑪

As part of the Science Talent Forsker Camp, 16 high school students got the chance to find out what it means to be a researcher and chemical engineer at DTU Chemical Engineering. Students got to work in real life laboratories at PROSYS research centre and experience large-scale production in the department's pilot plant facilities.

**12 October**

### THE HEMPEL FOUNDATION BOARD OF TRUSTEES VISIT COAST

The Hempel Foundation Board of Trustees visited the coating research facilities at DTU Chemical Engineering. The tour started with a poster presentation, which summed up the CoaST research areas, presented by Associate Professor Søren Kiil, followed by an introduction to the CoaST facilities conducted by Chief Consultant and Head of laboratories Claus E. Weinell. Next, a few hands-on case studies were presented at the experimental testing setups developed at the CoaST research centre.

**23-27 October**

### PROFESSOR GEORGIOS KONTOGEORGIS GAVE AN INVITED LECTURE AT CBTERMO 2017

Professor Georgios Kontogeorgis gave an invited lecture entitled 'Equations of State in Three Centuries—Are we closer to arriving to a single model for all applications?' at the IX Brazilian Conference CBTermo 2017.

**27 October**

### NEW HEAD OF WORKSHOP ⑫

We said goodbye to Head of Workshop Ivan Horst Pedersen after 28 years of service at the department. Ivan can look back at a job well done and pass on the torch to the next generation and successor Søren Vestergaard Madsen.

## NOVEMBER

**1 November**

### NEW HEAD OF PILOT PLANT

After 12 years as Head of DTU Chemical Engineering's Pilot Plant facilities, Lars Kiørboe retired. He can look back at an extraordinary development of the plant, and the department can look forward to its continuation under the leadership of Steen Larsen.

**23 November**

### CHEC ANNUAL DAY

On 23 November, CHEC invited their industrial partners and the entire CHEC group to share their newest developments and visions for the future. Approximatively 100 people participated. CHEC has grown a lot over the years with new and exciting research activities and 2017 was no exception, and ambitions for the future are still high.

**24 November**

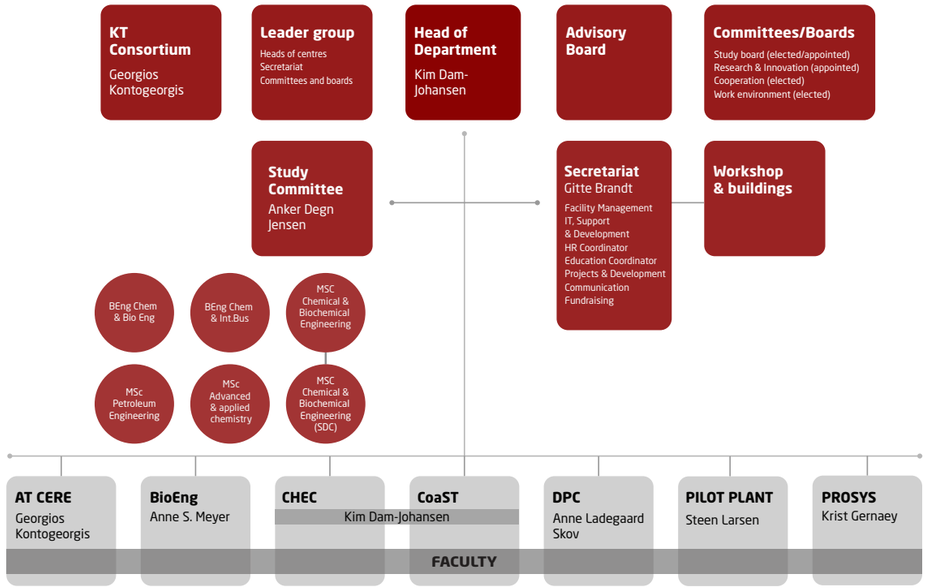
### DPC 13TH ANNUAL POLYMER DAY

Forty-six participants, both representatives from the Danish plastic industry and from the academic world, were gathered to share knowledge and research on polymers. The programme included presentations from a wide range of current polymer research, and the participants could leave DTU with new knowledge about many areas.

### FIVE DEPARTMENTAL SEMINARS

Throughout the year, we have hosted five departmental seminars with invited speakers from all over the world representing industry and academia. The seminars were well organized by Associate Professor Ioannis V. Skiadas and included lectures from Associate Professor Bradley D. Olsen from MIT, Andrea Saltelli from University of Bergen (UIB) and ICTA—Universitat Autonoma de Barcelona (UAB), Christos T. Maravelias from the University of Wisconsin, Madison, Dr. Pieter Schmal, Head of PSE Acadamic, and Professor Sandra Kentish from the University of Melbourne.

# ORGANIZATION




# ADVISORY BOARD

## LARS BANG

EXECUTIVE VICE PRESIDENT,
H. LUNDBECK A/S

"Implementing manufacturing of new medicines and continuously exploit 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."

## LARS PETERSSON

CHIEF OPERATING OFFICER,
EXECUTIVE VICE PRESIDENT,
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."

## BJERNE CLAUSEN

PRESIDENT & CEO,
HALDOR TOPSØE A/S

"Topsø'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."

## 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 an 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."



# RESEARCH CENTRES

DTU Chemical and Biochemical Engineering is home to seven research centres—each focusing on their area of expertise. Below you can get a quick overview of the centres and their respective research areas. To learn more about our research, recent results, or current projects, please visit www.kt.dtu.dk/research.

## AT CERE

Applied Thermodynamics, Transport Processes and Properties, Mathematical Modelling, Materials Science, Petroleum Technology, Enhanced Oil Recovery, $Co_2$ Capture and Gas Hydrates, Energy Resources.
Contact: Professor Georgios Kontogeorgis—gk@kt.dtu.dk—Phone: +45 4525 2859

## BIOENG

Bioprocess enzyme technology, Enzyme discovery, Enzyme kinetics, Enzyme engineering, Biocatalysis, Reactive separation technology, Biorefining, Bioconversion.
Contact: Professor Anne S. Meyer—am@kt.dtu.dk—Phone: +45 4525 2800

## CHEC

Catalysis, Inorganic chemistry, Combustion and flue gas cleaning, Diagnostics, Gasification, Pretreatment of biomass, Coatings, Pharmaceuticals.
Contact: Professor Kim Dam-Johansen—kdj@kt.dtu.dk—Phone: +45 4525 2845

## COAST

Sustainable coatings technologies including raw material engineering, smart formulation and production principles, application and testing, and tailor-made functionalities.
Contact: Professor Kim Dam-Johansen—kdj@kt.dtu.dk—Phone +45 4525 2845

## DPC

Polymer technology, Polymer chemistry, Rheology, Filament stretching rheology, Surface modification, Silicone polymers and elastomers.
Contact: Associate Professor Anne Ladegaard Skov—al@kt.dtu.dk—Phone +45 4525 2825

## PILOT PLANT

Designing and building large-scale plants, Unit operations, Industrial chemical processes, Operational experience, Design of components, Plant safety, Good Manufacturing Practice.
Contact: Steen Larsen—stelar@kt.dtu.dk—Phone +45 4525 2804

## PROSYS

Process Systems Engineering (PSE), Process Intensification and Integration (PII), Process Design and Control, Industrial Fermentation Technology, Biocatalysis, Microfluidics.
Contact: Professor Krist Gernaey—kvg@kt.dtu.dk—Phone: +45 4525 2970

# COOPERATING COMPANIES

**A**.P. Møller-Mærsk
Addifab
Agro Korn
Akzo Nobel
Alfa Laval
Aminord
Aquaporin
ARKEMA FRANCE
Arla Foods
ART photonics
AstraZeneca
At Sea Technologies
**B**&W Energy
Babcock & Wilcox Vølund
BASF
BAWAT
BAYER
Beyond Coffee
BiCT
Bio Aqua
Biofos
Bioneer
Biopro
BioProdict
BP
**C**alsep
Cargill
Carlsberg
CelluComp
ChemStream
Chevron
Chr. Hansen
Chreto
CILNorth
Ckj Steel
CLEA
c-Lecta
CMC Biologics
Coloplast
Conocophillips
COWI
CP Kelco
C-Tech
**D**aCoFi
Dansk Gasteknisk Center
DHI
DSM
DuPont
**e**Coast Marine Research
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ENGIE
Envidan
Esbjerg Farve- og Lakfabrik
Evocatal
Evonik
ExxonMobil
**F**CC Aqualia
FermBiotics
Fermentation Experts
FiberVisions
Firmenich
FLSmidth
Foss
FreeSense
**G**ASSCO
GASSNOVA
GDF-SUEZ
GEA Process Engineering
Gelest
Genencor
Givaudan
GlaxoSmithKline
GLYCOM
Grundfos
**H**. Lundbeck
Haldor Topsøe
Hempel
Hempel Foundation
Hess
HOFOR
Hortimare
Huntsman Polyurethanes
Hwam
Højmarks Group BHJ
**I**BUS Innovation
**J**ANSSEN pharmaceutica
**K**alundborg forsyning
KBC
KMC
**L**EAP Technology
LEGO
Lentikats
Leo Pharma
LevOss
Lihme Protein Solutions
Linde
Liqtech International
LPS
Luxcel
**M**aersk Oil
MAN Diesel & Turbo
Melissa
Meneta
Microfluidic ChipShop
Micronit
Mitsubishi
MOL
Morgenfruerne
**N**anomyP
National Oilwell Varco
Nestle Jacobs
Nordic Bioenergy
Nordic Sugar
Nordisk Tang
Nova Pangea
Novo Nordisk
Novozymes
NxPAS ApS
**O**cean Rainforest
OceanBasis
**P**articleTech
Petrobras
Pfizer
PHX Innovation
Process-design
Processium
ProSim
Prozomix
**Q**-Interline
**R**adiometer
Rambøll
Rockwool
RWE
**S**BM Offshore
Scheider Electric Software
Schlumberger
Schneider Electric
Shell
Sigma Aldrich
Sika
Sinopec
Solvionic
S-PACT
SpinChem
Statoil
Supren
Syngenta
**T**eknologisk Institut
Tetra Pak Packaging Solutions
TOTAL
Trioplast
Trojan technologies
**U**nibio
Unicense
UNILEVER
Union Engineering
**V**eolia Krüger
**W**acker
Welltec
**X**ellia Pharmaceuticals
**Ø**rsted

# RESEARCH & INNOVATION

From left, Student Dennis Skov Kloth on the controls together with Postdoc Susana Raquel Melo de Almeida, Associate Professor Nicolas von Solms, and Associate Professor Philip Loldrup Fosbøl.
A new technology is being developed which allows for low energy consumption during biogas upgrading for production of green $CO_2$ ($BioCO_2$) and biomethane. The absorber being controlled will be extended and made mobile for biogas upgrading at a waste water facility and at manure sites in Denmark.

Photo: Thorkild Christensen

Associate Professor Ioannis Skiadas and PhD student Anna Lymperatou in front of a plant for pilot scale organic synthesis made of glass and stainless steel.

Photo: Thorkild Christensen

### The AMMONOX project

The research within pretreatment of biomass for energy production was carried out at the PILOT PLANT centre and at the BioEng centre, DTU Chemical Engineering, as part of the AMMONOX (Ammonia for Enhancing Biogas Yield & Reducing $NO_x$) project funded by Energinet.dk, ForskEL. The Danish Gas Technology Centre, Nordic Bioenergy ApS, and Envidan A/S were partners in the project, which ran from 2013-2017.

The energy potential of manure can be significantly increased through a contemporary chemical engineering twist to an abandoned agricultural technique. A collaboration between Associate Professors Ioannis Skiadas and Hariklia Gavala and PhD student Anna Lymperatou has resulted in a three-fold increase in the amount of methane produced from the solid fraction of swine manure, under lab conditions.





# Farmers' know-how revived for bioenergy

Methane is a highly desirable product as it can be directly stored, transported, and distributed in the Danish natural gas system. Unlike the lab setup in the project, the existing digesters in the Danish biogas industry are built for liquids and are not optimal for pumping of solids.

*"Due to the limited amounts of solids we can pump in the existing digesters, we cannot achieve a 200 per cent increase in the methane production from the full-scale biogas plants as we did in the lab, but something like 25-30 per cent does seem realistic. This would benefit the economy of this industry, and also be an important contribution to the realization of the ambitious Danish bioenergy policy,"* Ioannis Skiadas comments.

## Transforming an old farmer's practice to an industrial process

One of the challenges in relation to the use of manure for bioenergy purposes is its high content of ammonia from the animals' urine. The project, a collaboration between the PILOT PLANT and BioEng centres, turns this problem into an advantage by bringing the ammonia to use. Through their innovative Aqueous Ammonia Soaking (AAS) technique, fibres from straw and other biomass products are soaked in ammonia. The process greatly enhances the methane yield, as a much higher proportion of this so called ligno-cellulosic biomass becomes available for methane generation.

*"In a way, the technique mimics an old farmer's practice. Half a century ago, it was common to apply gaseous ammonia on straw piles. Not to produce bioenergy, but to make this cheap feedstock more available to be digested by cows. We are doing a similar thing as a pretreatment for bioenergy production, only without involving cattle. After the process, the ammonia is removed under strictly controlled conditions. Then, we let microbes digest the ammonia-soaked biomass and convert it into methane,"* explains Ioannis Skiadas.

The old farmer's practice was abandoned—and even forbidden—for environmental reasons, as it transpired that the airborne release of ammonia had several harmful effects.

*"In our context, the ammonia will of course not be released. It is captured and recycled for further soaking."*

## Significant contribution to energy policy

Currently, only 10 per cent of the swine manure in Denmark is used as feedstock for biogas production. The remaining 90 per cent is dispersed on fields. On the upside, this does contribute to fertilizing, but also causes smell issues and other environmental concerns. Thus, it is a key energy policy target to increase the proportion of manure used in biogas production.

*"Progress on increasing the proportion of manure used for bioenergy has been halted by the lack of economic incentives for the farmers and biogas plant owners. When the methane yield is increased, this incentive becomes higher,"* says Ioannis Skiadas, further emphasizing:

*"If all manure from swine, cattle, and poultry was utilized, this would trigger a many-fold increase in the production of biogas in Denmark. This would be a huge contribution to achieving the long-term renewable energy targets, while also solving several environmental challenges involved in the current use of manure."*

Experimental proof of concept for enzymatic $CO_2$ conversion to $CH_3OH$ has been achieved via diligent experimental work and enzyme kinetics modelling.

Photo: Thorkild Christensen

- Fauziah Marpani was awarded a prestigious scholarship from the Ministry of Higher Education Malaysia and Universiti Teknologi MARA (UITM). Fauziah did her PhD work at DTU Chemical Engineering on 'Enzyme Immobilization and Redox Enzyme Kinetics in Membrane Bioreactor Systems'. After returning to Malaysia, she has resumed her post as a senior lecturer at UITM.

- The research continues at DTU with two new PhD projects. Christian Førgaard Nielsen will carry out 'Discovery and Engineering of new Enzymes for Efficient Enzymatic Conversion of $CO_2$'. His project is funded by BioValue SPIR and DTU Chemical Engineering. Zhibo Zhang investigates 'Use of Ionic Liquids and Support Materials for High Performance Enzymatic Conversion of $CO_2$ into Formic Acid and Formaldehyde'. This project is sponsored by the Institute of Process Engineering, Chinese Academy of Science, and DTU Chemical Engineering. Both of these new PhD projects are designed to bring conversion of $CO_2$ into useful products via enzyme-catalysis even closer to implementation.

Increased atmospheric levels of carbon dioxide, $CO_2$, are commonly known as the number one cause of global warming and climate change. Efforts at the BioEng centre aim at alleviating the $CO_2$ increase by using $CO_2$ as a feedstock for production of fuel and chemicals. An enzyme-catalysed system is used at the centre to convert $CO_2$ into methanol ($CH_3OH$), a useful fuel, while producing either gluconic acid or xylonic acid at the same time. Both gluconic acid and xylonic acid are categorized by the US Department of Energy to be among the top 30 potential basic precursors relevant for synthesis of high value chemicals and fuels.



# Enzymes convert $CO_2$ into high-value products

$CO_2$ is an end product of many naturally occurring and industrial processes. Burning of fossil fuels in thermal power plants as well as facilities like cement and steel factories contribute heavily to $CO_2$ emissions. However, both the carbon and the oxygen in $CO_2$ are potential feedstocks for a wide range of products including fuel, food, and precursors for polymers and other valuable chemicals.

*"At BioEng we look into enzyme-catalysed processes that can utilize $CO_2$ in new processes. Enzymes are able to work under mild conditions. i.e. normal pressure and moderate temperatures, and can convert $CO_2$ in the air directly into formic acid and other chemicals including methanol,"* explains Fauziah Marpani. She recently handed in her PhD thesis at BioEng, DTU Chemical Engineering.

As the enzymes do not require high temperatures and pressure, the chance of creating sustainable solutions with low energy input is high. Further, the enzymes are highly specific, meaning they yield the desired end product without producing other substances.

## Three different enzymes are required

No single enzyme is able to reduce $CO_2$ all the way to $CH_3OH$. Three steps are needed, each catalysed by a different enzyme. In Fauziah Marpani's setup, three enzymes are applied which can all use the same cofactor for the reducing equivalents' electron supply, namely NADH (nicotinamide adenine dinucleotide). NADH is found in all living cells, and serves as a reducing agent to a wide range of enzymes.

The need for NADH in the enzymatic process is high. Since each of the three steps requires NADH, the total (molar) consumption is three times the amount of the methanol produced.

Therefore, it is really good news that BioEng has managed to design a dual system, where NADH is regenerated synchronously with its consumption in the enzymatic $CO_2$ conversion process.

*"Enzymatic conversion of $CO_2$ to useful products is a new approach to reduce $CO_2$ levels that simultaneously provides a sustainable supply of high demand products. I really do envisage a future, where industrial $CO_2$ emitters have devices with immobilized $CO_2$ converting enzymes installed in their exhaust pipes so that they can both reduce emissions and at the same time create value from the $CO_2$ exhaust streams by producing useful chemicals. Our immediate aim is to generate robust enzymes supporting this scenario,"* says Professor Anne S. Meyer, Head of BioEng.

## Reactions run in parallel

In the system, $CO_2$ is reduced into methanol ($CH_3OH$) via two intermediate products, formaldehyde (CHOH) and formic acid (CHOOH). Each step requires NADH, which is oxidized to NAD+. To avoid loss of the expensive NADH co-factor, and at the same time generate value, Fauziah Marpani regenerates NADH by running a second reaction in parallel. This reaction is either the oxidation of xylose to xylonic acid or the oxidation of glucose into gluconic acid.

The coupled reactions demonstrated a high biocatalytic productivity.

*"The production of xylonic acid and gluconic acid provides a valuable addition to the important regeneration of NADH. This highly useful by-product increases the chances of converting $CO_2$ into methanol in an economically feasible way,"* says Fauziah Marpani.

*"We have now passed the proof of concept stage for enzymatic $CO_2$ utilization. In 2017, via Fauziah Marpani's PhD work, we thus attained reaction optimization of the methanol formation step by designing synchronous enzymatic reduction and co-factor regeneration via kinetic modelling. The next priority is to further improve the biocatalytic cascade reaction by improving the enzymes. We also plan to calculate the energy requirements, including determining the thermodynamic equilibria of the reactions in the designed reaction cascade,"* says Professor Anne S. Meyer, Head of BioEng.

Associate Professor Kaj Thomsen in front of the high temperature cell made from titanium. The solubility of iron, lead, and zinc sulfide in water was measured at temperatures up to 175 °C in this equipment. Titanium was chosen in order to avoid corrosion.

Photo: Thorkild Christensen

- NextOil is a CERE project, which means that it is shared between DTU Chemical Engineering, DTU Chemistry, and DTU Civil Engineering. The AT CERE research centre at DTU Chemical Engineering is the main partner in NextOil.
- NextOil consisted of three work packages: WP 1: Rock mechanics, WP2: Hydrocarbon reservoir fluid, and WP3: Scaling.
- The project is funded by the Danish National Advanced Technology Foundation (DNATF/HTF) as well as by Maersk Oil and DONG.
- The project ran from November 2012 to June 2017.

Salts play a major role in fields from oil production to biological processes. In AT CERE, a databank with 173,649 experimental data points for 342 different salts has been compiled from 3,167 scientific papers and reports.

Oil reserves are decreasing, pushing extractors to look for 'the black gold' at unorthodox locations deep in the ground. This causes problems, partly because—as the NextOil project at AT CERE has shown—it is a lot more complex to measure salts and other chemical elements in the deep reservoirs than previously assumed. It is important to know the solubility limits of the salts to avoid clogging of the pipes due to precipitation.

# Oil under pressure

It is hardly a secret that oil is a scarce resource. This poses several challenges: One is to develop new, sustainable energy resources to replace oil in the long run. Another is to find better ways to reach oil reserves embedded in less accessible reservoirs.

NextOil—which stands for 'New Extreme Oil and Gas in Denmark'—has been on the case since its start in 2012. The project aims to reduce the technical and economic risks in developing oil and gas from so-called HP/HT (High Pressure/High Temperature) reservoirs. Located deep underground, HP/HT fields have temperatures above 150 degrees Celsius and pressures of more than 700 bar, making the conditions of extraction troublesome.

*"In HP/HT areas there are sulphide salts that are not found in places where pressure and temperature are moderate. And these salts can pose a problem for the production. If the solubility limits of these salts are known as function of temperature and pressure, it is possible to adjust the process conditions in such a manner that precipitation on the walls of the pipes is avoided. This would not be a big problem if we had easy and effective methods for measuring them—but, unfortunately, we do not."* says Associate Professor Kaj Thomsen, who is heading the NextOil project at DTU Chemical Engineering's research centre AT CERE.

The measurements of the solubility of sulphide salts that have been made earlier in the history of chemical engineering do not really show what they were supposed to. In fact, they are so imprecise that they are misleading, and a big part of NextOil has been to develop a theoretical foundation for better measurements. Based on the new measurements performed in the NextOil project, it is possible to improve current thermodynamic models, such as the Extended UNIQUAC model used in the ScaleCERE software so that they are able to predict the precipitation of sulphide salts. Such models can help to determine suitable process conditions to avoid clogging of pipes by precipitation. Alternatively, such models can be used for determining the feasibility of a certain production.

*"We have established that earlier measurements of the solubility of zinc, lead, and iron sulphide are very inaccurate. We used a tool called ICP-OES (Inductively Coupled Plasma Optical Emission Spectometry) that can be used to measure very small amounts of chemical elements. Our analysis reveals that the deep reservoirs are more complex and unknown than previously thought, and this is vital knowledge when advancing the production in HP/HT fields,"* says Kaj Thomsen.

## Industry wants knowledge

The NextOil research findings thus lay a foundation for further advancement: If the industry extracting the oil from HP/HT reservoirs can stop making scientifically unwarranted assumptions based on previous inaccurate measurements, then economic losses and technical trouble can likely be avoided. And new, more precise, measuring methods can be allowed to see the light of day.

*"The industry is very interested in our findings and what they can mean for the future of HP/HT extraction. We have put our finger on some problems that need to be solved. There have been incidents, for example in the UK part of the North Sea, where HP/HT oil fields have gone out of hand because the extractors were not conscious about some of the potential problems. The industry has an immense interest in knowing what they are dealing with,"* says Kaj Thomsen.

Many of the HP/HT reservoirs are found offshore, including in the North Sea and the Gulf of Mexico. The oil extracted from these fields is not only utilized as fossil fuels but also to make materials, such as plastic. Development of oil production in these areas comes with a risk—but they can be highly rewarding if done on a sound foundation of knowledge.

## A sustainable angle

Not only the oil industry can benefit from the results of NextOil. The project also points us towards more effective ways to access greener energy resources:

*"In a number of years' time, the oil will be gone. But another, more sustainable, way to produce energy is geothermal energy sources—the heat that is already stored in the Earth. Our research applies to this area as well,"* says Kaj Thomsen.

Geothermal energy is already used to generate district heating in Denmark, for instance at the Amagerværket CHP plant in Copenhagen and at two different plants in Jutland. It is still on a small scale, in Denmark as well as internationally, but the potential will need to be developed for the energy needs of tomorrow:

*"Just like in oil fields, there is likely sulphur and other elements in geothermal plants that we need to measure as precisely as possible in order to optimize the extraction process. The knowledge gained through NextOil is useful at both places,"* says Kaj Thomsen.

The elastomer properties are tested in cyclic deformations mimicking the operation of the dielectric elastomer. Dielectric elastomers are usually very soft and flexible and can easily be deformed several hundred per cent.

Photo: Thorkild Christensen

- Since 1918, DTU has awarded the doctor technices degree to more than 200 recipients. The award of the doctorate is based on a thesis demonstrating the author's considerable academic insight and maturity, and that the thesis has brought science an important step forward.
- Anne Ladegaard Skov is the seventh woman ever to receive a doctoral thesis from DTU.
- In 2017, Anne Ladegaard Skov received the Statoil Prize of DKK 100,000 as a personal prize for her internationally recognized research within the field of dielectric elastomers.
- The studies behind the thesis was conducted over a period of about five years, and seven PhD students, five postdocs as well as scientists from Danfoss PolyPower and DPC colleagues have been contributing to the research of the thesis project.



At the DTU Commemoration Day 2017, Anne Ladegaard Skov was awarded the Doctor Technices degree for her research in dielectric elastomers—or, popularly speaking, artificial muscles.



# Anne Ladegaard Skov was granted the degree of Doctor Technices

On 28 April 2017, Anne Ladegaard Skov from DTU Chemical Engineering officially achieved the degree of Doctor Technices at the annual DTU Commemoration Day. In March, she defended her thesis on research into so-called dielectric elastomer transducers, which in layman's terms can be described as 'artificial muscles'. Anne Ladegaard Skov's thesis provides the most thorough insight into the potential of dielectric elastomers to date within the scientific area.

More specifically, dielectric elastomers are rubbery materials which expand similarly to natural muscles when exposed to an electric field.

*"Dielectric elastomers consist of a thin sheet of elastic polymer (an elastomer) that is squeezed between two flexible electrodes. When an electric voltage is applied to the electrodes, the two opposing electrodes will attract each other. This results in a thinning of the elastomer as well as an expansion in its area. When the electric voltage is detached, the material will return to its original form,"* Anne Ladegaard Skov explains.

Artificial muscles made from elastomers can be used for pumps, valves, robots, actuators, generators, sensors, and energy harvesters.

Mainly funded by Innovation Fund Denmark and industry, Anne Ladegaard Skov's research group has found that silicone-based elastomers are the best material for artificial muscles, as this silicone is more durable, reacts quickly, and can handle cold as well as warm environments.

*"The specific subject of my doctoral thesis was improvement of properties of silicone-based dielectric elastomers with special focus on design guides towards electrically, mechanically, and electro-mechanically reliable elastomers, focusing on long-term reliability of the dielectric elastomers and how to achieve this by means of careful elastomer design,"* Anne Ladegaard Skov says.

## Soft robotics and harvesting wave energy

The technology of dielectric elastomers has gained significant impact over the last couple of years with so-called soft robotics being discussed as a paradigm-changing technology. Dielectric elastomers are one technology among many capable of fulfilling aspects of the soft robotics era but dielectric elastomers hold great promise since it is inherently flexible and can be stacked and folded into an unlimited number of configurations. New technologies to produce even thinner films, and thereby more efficient dielectric elastomers, have seen the light of day. These processes, however, put vast requirements on the properties of the elastomer reactants and the elastomer itself. This challenge is also something that the research group is actively involved in.

Novel constructions of dielectric elastomers have also been explored, leading to soft wave energy harvesters (WECs) with unprecedented efficiencies. Building on the knowledge gained from her research, Anne Ladegaard Skov has participated in the SBM France-funded project Wave Energy Converter.

In WEC, a long tube of dielectric elastomers is placed offshore and is then deformed by the motion of the ocean waves. These deformations can be transformed into electric energy.

*"We are dealing with very large wave powers that expand whatever material we use, and this requires a material that is both lightweight and flexible—elastomers are ideal for this purpose,"* Anne Ladegaard Skov says.

## The future of the science of artificial muscles

On top of these achievements, Anne Ladegaard Skov has also been elected as the new president for the non-profit association for promoting the scientific and technological advancement of transducers and artificial muscles, the EuroEAP Society. This goes hand in hand with her extensive research into dielectric elastomers which, as stated above, was the basis of her doctoral thesis.

*"The coming four years will be extremely interesting from a commercial point of view with electro-active polymers entering more and more novel products as well as there still are multiple fundamental aspects to be covered in order to fulfil the full potential of the technology. A lot of focus will be put on establishing fruitful collaborations between scientists and companies during the coming years,"* Anne Ladegaard Skov says about her new role as President of EuroEAP.

Professor Anker Degn Jensen and Senior Researcher Brian Brun Hansen at the flexible setup that allows studying all the steps in the catalytic cleaning of diesel exhaust gas.

Photo: Thorkild Christensen

### The NEXT project

The 'Next generation exhaust gas cleaning technologies for diesel vehicles' (NEXT) project ran from April 2013 to August 2017. The partners were Haldor Topsøe A/S and DTU Chemical Engineering with funding from the partners and Innovation Fund Denmark. The innovation fund provided DKK 9.6 million of the total budget of DKK 19.3 million. The project involved two research centres at DTU Chemical Engineering—PROSYS and CHEC.

Close-up of a soot filter. In NEXT it was investigated how a catalyst could be added to such a filter to enable even more efficient soot removal and simultaneous $NO_x$ removal. Photo: Thorkild Christensen.

# Smarter cleaning technologies for diesel vehicles

Health concerns have led to still more stringent authority regulations of emissions from diesel-driven vehicles. A five-year collaboration between Haldor Topsøe A/S and DTU Chemical Engineering and funded by Innovation Fund Denmark has taken significant steps towards more efficient treatment of diesel exhaust gas through both optimized catalytic formulations and new innovative combined units.

Haldor Topsøe, a world-leading catalysts manufacturer, has supplied catalysts for the automotive industry for some time, but was keen to improve the catalysts further in order to stay competitive.

*"The main harmful compounds in diesel exhaust gas are soot particles, unburned hydrocarbons, nitrogen oxides ($NO_x$), and carbon monooxide (CO). Currently, each of these have a dedicated treatment sub-system. CO and hydrocarbons are catalytically oxidized to $CO_2$ and water by a diesel oxidation catalyst (DOC). The soot particles are caught and converted to $CO_2$ in a diesel particulate filter (DPF), while the $NO_x$ is catalytically reacted with ammonia ($NH_3$) to $H_2O$ and $N_2$,"* explains Professor Anker Degn Jensen, head of the project.

Research in the NEXT project (Next generation exhaust gas cleaning technologies for diesel vehicles) has looked into low noble metal content DOCs and combined soot and $NO_X$ removal. Further, optimal reactor configurations for $NH_3$ control, new model based $NO_x$ emission control strategies and in-situ transmission electron microscopy (TEM) studies of the catalytic conversion of soot have been investigated.

## Optimal size of catalytic particles identified

The project has demonstrated that the DPF and the catalytic $NO_x$ treatment may be combined into a single unit using a mixture of vanadium and cerium oxides.

*"The possibility of combining two catalytic units into one is highly welcomed by the automotive industry. Space and weight is always an issue on a vehicle, and when two systems are combined, space is saved. Further, the new compact cleaning unit reaches the required operating temperature faster thereby limiting emissions,"* says Brian Brun Hansen, Senior Researcher at DTU Chemical Engineering.

Another important finding relates to the optimal size of catalytic nano-particles in the diesel oxidation catalyst. In NEXT, the optimal particle size for platinum (Pt) particles in a $Pt/Al_2O_3$ catalyst for oxidation of CO, propene ($C_3H_6$), and NO was found. Platinum is an effective catalyst in a range of reactions, but it is also an expensive component, which makes it even more relevant to identify the optimal use. Further, the finding has implications for other catalyst materials.

As a rule of thumb, small catalytic particles are desirable, since small particles equals a large surface area for the reaction to take place on. However, NEXT studies of the $Pt/Al_2O_3$ system show that 2-4 nanometres is the optimal size for the Pt-particles, balancing maximal surface area and optimal catalyst surface topology (expressed as terrace, edge, and corner atoms).

## Implemented by Topsøe

The project also involved collaboration between two research centres at DTU Chemical Engineering—PROSYS and CHEC. At PROSYS, Associate Professor Jakob Huusom worked on developing models for the cleaning units and applying these models in advanced control algorithms.

*"The research performed includes well-controlled small-scale kinetic powder experiments, but also monolith test on a medium-size engine, while Topsøe has tested in their full-scale engine lab,"* says Senior Researcher Brian Brun Hansen.

Part of the results in NEXT have already been implemented in Topsøe's heavy duty diesel and stationary catalyst businesses, while other require further work before industrial implementation.

A very important result of NEXT is that four PhD and a number of MSc students were educated under the NEXT umbrella.

*"When we started NEXT, there were practically no graduates in automotive catalysis. The project has changed the scene completely, with some 15-20 new BSc and MSc graduates plus the four new PhDs. We now have a genuine research environment within this important topic,"* says Anker Degn Jensen.

The Topsøe automotive and stationary DeNOx catalyst businesses were acquired by Umicore in June 2017 and are expected to develop further with a base in Denmark.


PhD student Xueting Wang performing real time levelling studies on antifouling coatings with our new optical 3D profilometer.

Photo: Thorkild Christensen

## Vision

CoaST is a globally leading centre for research, innovation, and education in sustainable coatings technologies.

## Mission

- Establish a strong research, innovation, and education environment at DTU supported by an extended global network to leading research and development groups.
- Develop new and improved methods and technologies for the formulation, testing, characterization, production, and application of coatings with improved sustainability profiles.
- Establish a platform for cooperation among stakeholders of coating technologies, i.e. universities, raw material suppliers, formulators, producers, applicators, and/or end users.
- Attract and train highly skilled students, engineers, and researchers to the field of coatings.

Sustainable coatings technologies, including raw material engineering, smart formulation, production principles, application, testing, and tailor-made functionalities, is the core of the research, educational, and innovative activities at the new research centre CoaST- The Hempel Foundation Coatings Science and Technology Centre, located at DTU Chemical Engineering.





# Coatings for a better future —new research centre in coatings science and technology

CoaST was established in January 2017 following a generous donation by the Hempel Foundation with the vision of establishing a globally leading centre for coatings related activities. The donation was given as a result of a long-time productive collaboration on coatings technologies between the Hempel Foundation and the CHEC research centre at DTU Chemical Engineering.

"*We are excited with the opportunity to expand our research within coatings, which for the past 17 years have been an integrated part of the CHEC research centre here at DTU Chemical Engineering. Throughout the years, we have gained a high level of expertise within the area of coatings, resulting in several significant results. Now it is time to grow the field. CoaST will primarily draw on the best professional expertise in both academia and industry, and we seek to make a profound difference for not only the coating industry but also the environment,*" says Kim Dam-Johansen, Head of DTU Chemical Engineering and Head of CoaST research centre.

This long-term commitment from the Hempel Foundation gives CoaST the premises of establishing a highly proficient research centre, with unique state-of-the-art facilities and highly qualified personnel.

### From raw materials to application

Advanced functional coatings are used in many parts of various industries, applied onto different types of surfaces and exposed to variable environmental parameters, such as temperature, humidity, light exposure, and salinity. This means that a coating needs to be tailored, in terms of composition and functionality, in order to perform as desired for a specific application. For instance biofouling and corrosion control is required for steel structures on ships, offshore platforms and pipelines, while passive fire protection is required for buildings in order to provide longer escape times during a fire.

This year, in open dialogue with internal and external, academic, and industrial partners, and using a holistic approach, CoaST has identified relevant research fields for coating science and technologies and defined the strategic focus area to:

- Anticorrosive coatings
- Chemical and abrasion resistant coatings
- Coatings for passive fire protection
- In-line coating production
- Erosion resistant blade coatings for wind turbines
- Fouling control coatings
- High-pressure, high-temperature coatings
- Thermal insulation coatings

CoaST inherent research approach is based on chemical engineering disciplines, as follows:

- Formulation (coating) expertise
- Pilot plants for coating exposure
- Materials, interfaces, surfaces
- Transport processes
- Reaction engineering
- Mathematical modelling

### A new generation of engineers

Besides research and innovation, CoaST provides high-quality, industrially relevant education in the field of functional coatings, by contributing to teaching and supervision of BSc, MSc, and PhD students enrolled at DTU. Both teaching and research are conducted in close collaboration with industrial companies, ensuring connection to present day industrial activities. The close link between research, industry, and education supports the mission of attracting and training the new generation of expert engineers within the field of coatings.

The tube-in-tube reactor, operated in low dispersed flow regime with flow ramp, is able to determine the full kinetic profile for oxygen-dependent enzymes, used in the synthesis of a wide variety of chemicals.

Photo: Thorkild Christensen

### The BIOOX project

The European BIOOX project has developed tools for implementation of bio-catalytic synthesis and oxidation of alcohols. New bio-catalytic oxidation reactions are in high demand, as they may replace more hazardous and less environmentally benign industrial oxidation methods.

Overall coordinator was the University of Manchester, with DTU and University of Stuttgart as the other academic partners. Industrial participants: BASF SE, CLEA Technologies BV, Prozomix Ltd., C-TECH Innovation Ltd., BiCT srl, Bio-Prodict BV, and Firmenich SA.

The BIOOX project began in September 2013. The project was formally concluded in September 2017, but cooperation between the partners continues. The project received funding from the European Union's Seventh Framework Programme for research, technological development, and demonstration.

Pleasant fragrances and flavours are all around us, and often need to be synthesized in industrial processes. It is good news for this industry that enzymes can be efficient bio-catalysts for many of the key reactions involved. This will enable cheaper and more environmentally benign production.





# A scent of almond with a hint of enzyme

A project at the Process and Systems Engineering Centre (PROSYS) has contributed to this end through a major EU-funded project, BIOOX, with a range of European academic and industrial partners.

Traditional chemistry will often produce the end product in slightly different molecular structures of which only one has the desired smell or taste. In some cases, the other versions can be tolerated. However, more often they will need to be removed. This implies waste generation and higher costs. Enzymes are typically stereo or regio-selective, meaning they only yield the molecule with the exact desired structure.

## Industry craves faster reactions

*"Many of the fragrances and flavours in high demand can be created through oxidation reactions. Numerous enzymes are capable of catalysing the desired oxidations. This is the focus of the BIOOX project,"* says Asbjørn Toftgaard Pedersen. Today he is with Novozymes, but he recently completed his PhD in PROSYS. His PhD project 'Oxygen Dependent Biocatalytic Processes' was supervised by Professor John M. Woodley as a part of BIOOX.

*"If industry is to replace the present chemical pathways with enzymatic reactions, it will be crucial that the enzymes can perform their task robustly at a sufficiently high speed,"* says Professor Woodley.

He adds, *"BIOOX has been hugely successful, resulting in new technology as well as new enzymes and reactions. The latest technology from the project will form the basis of future projects at PROSYS and DTU Chemical Engineering."*

Several of the industrially relevant enzymatic reactions require oxygen. This is of course normally delivered from air, but the story does not end here, Asbjørn Toftgaard Pedersen explains:

*"Unfortunately, the transfer of oxygen from air to an aqueous solution is notoriously slow at ambient conditions. One way to increase the speed is through vigorous agitation and aeration, but this adds to costs and also sets a limit to the maximum productivity of the reactor. Another possible solution is to develop enzymes that are able to function efficiently at the low oxygen concentrations typically found in industrial reactors. The project has combined our own chemical engineering approaches with the protein engineering and directed evolution approaches of our colleagues at the University of Manchester."*

## Plant protection by smell

As the many different enzymes have different properties and characteristics, there is no single universal way to achieve the optimal reaction conditions.

*"Probably more important than the various recommendations for different reactions is the development at PROSYS of a new experimental setup. We have built a so-called tube-in-tube reactor (TiTR). This setup is capable of performing fully automated kinetic characterization of oxygen-dependent enzymes. The method enables fast characterization of enzyme variants developed through protein engineering. Thus, it will hopefully contribute to further advances in the use of enzymes as biocatalysts,"* says Asbjørn Toftgaard Pedersen.

Besides synthesis of well-known scents like almonds or roses, and tastes like vanilla, enzymes can play a role in less apparent contexts. An example is a new trend in protecting gardens and crops from pests:

*"Rather than spraying your plants with traditional insecticides, you can generate smells that will discourage the insects,"* says Asbjørn Toftgaard Pedersen.

Further, the same challenges facing the production of fragrances and flavours can be found in a range of other oxygen-dependent enzyme reactions. These include synthesis of pharmaceuticals, agro-chemicals, and monomers for polymer production.

# Impressions from the Annual Meeting

*"It's great to see and hear that the way forward for a sustainable consortium has been found, and what we've seen at the conference is that there's thought given to continued research areas. I think this was the first opportunity for us to see how this was going to evolve in the future with my expectation that we will have the opportunity to have a role to play in shaping that future"*

**Patrick Piccione, Syngenta Fellow Group Leader & member of the KT Consortium Advisory Board**

*"There's no way we can be experts in every area and therefore we want to collaborate with universities such as DTU, and specifically KT Consortium is great for that. We've been in this consortium for almost 25 years—so the history goes back"*

**Nevin Gerek, Principal Research Engineer at Schneider Electric**

*"We cannot find one company or one university that is big enough to develop everything, so we need to have cooperation, which means we can go faster and more efficiently towards solutions. So, cooperation is the key"*

**Denis Lancon, Academic and Collaborative Research Coordinator at Total**





# Summary of the KT Consortium Annual Meeting 2017

From 6-8 June 2017, 54 delegates from industry and academia from around the world gathered for a three-day Annual Meeting in Elsinore north of Copenhagen. The focus of the conference was on how to ensure that research and innovation go hand in hand with the future needs of society.

The Annual Meeting started in Lyngby and following a workshop and a tour of the large pilot plant of DTU Chemical Engineering, the group commenced their journey north towards the historic Marienlyst conference centre in Elsinore and two days of presentations, poster sessions, and discussions. At the Annual Meeting, the new head of the KT Consortium was announced: Professor Georgios Kontogeorgis will be leading the consortium succeeding Professor Rafiqul Gani, who for many years was the head of the CAPEC centre and consortium (predecessor of KT Consortium). Fortunately, Professor Kontogeorgis is no stranger to managing and developing large consortia. With his many years as Head of AT CERE and later the Centre for Energy Resources Engineering (CERE), he is an experienced networker who has succeeded in building a large and strong consortium. However with the KT Consortium, Professor Kontogeorgis will not be starting from scratch. The new consortium builds on the work performed by the CAPEC consortium which has existed since 1997. Consequently, most of the current members have been affiliated for almost as long. Therefore, many of the industry members were interested to see where the new reorganized consortium will be heading.

## Discovering mutual interest and potential

During the discussions at the Annual Meeting, it was clear that the interests of the industry members vary significantly. It is a diverse group. Currently, the KT Consortium consists of 16 companies from the chemical, food, simulation, biotech, and pharmaceutical sectors. Yet, this did not deter the many members from finding common interest in some important issues that concern them all. As such, the discussions mostly centred around thermodynamics and related property prediction as well as process design and synthesis. Modelling and simulation were also key interest areas for the companies, as most of the industry members are particularly interested in the popular Integrated Computer Aided System (ICAS) software developed over the years by the research group led by Professor Rafiqul Gani.

*"It was clear from the Annual Meeting that the companies would like to see these ICAS/software activities continued and enhanced. In time, we will see whether some of these companies may become interested in other tools and research projects provided by the Department of Chemical and Biochemical Engineering"*, says Professor Kontogeorgis who is also no stranger to the challenge of finding common ground in a complex constellation of diverging interests.

## Cooperation is key

Aside from the ICAS software, one interest that all companies seemed to have in common was in keeping up with the newest knowledge. Denis Lancon is a 'Coordinateur Recherches Universitaires et Coopératives' at Total as it beautifully states in French—a title which Lancon seems to fully embody in his visit to the KT Consortium Annual Meeting. To him, the key to acquiring new knowledge does not revolve around having the most resources—instead it is a question of being able to cooperate with others outside your own organizational boundaries.

## A rare opportunity

The consortium has been around for a long time and many of the original members still prioritize travelling many kilometres from their respective countries to Denmark each year to participate in the Annual Meeting. Apart from KT Consortium members getting the tools that they need in their work, another rare opportunity has also presented itself for people who are not member of the consortium: All presentations and posters from this year's conference have been made available online.
Go to the KT Consortium website at http://www.kt.dtu.dk/english/research/kt-consortium

# EDUCATION

**STUDENTS WORKING IN DTU CHEMICAL ENGINEERING'S PILOT PLANT**
Practical courses, student and research projects are running all year round in the large Pilot Plant facility. We have more than 30 different large-scale equipment installations at our disposal, representing all typical chemical and biochemical unit operations, allowing the students to combine theory and practice and to simulate industrial scale behaviour.

Photo: Christan Ove Carlsson

# 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, catalysis, computer modelling, process and product design.

# COURSES 1 SEPTEMBER 2016 – 31 AUGUST 2017

## PHD COURSES

28901 Advanced Computer Aided Modelling
28904 Polymer Physics
28905 Advanced Topics In Process Systems Engineering
28908 Rheology of complex fluids
28909 Thermodynamics Models, Fundamentals and Computational Aspects
28917 Statistical Thermodynamics for Chemical Engineering
28924 Process Engineering Laboratory
28927 Advanced Topics in Process Technology
28928 Electrolyte Solution Thermodynamics
28930 Advances in Chemical and Biochemical Engineering
28931 Biorefinery and Sustainability

## SINO-DANISH CENTER (SDC) COURSES

88700 Industrial Reaction Engineering
88701 Transport Processes
88703 Laboratory Experiments
88704 Progress in Research
88705 Process Design—Principles & Methods
88707 Energy and Sustainability
88708 Green Chemical Engineering
88711 Industrial BioReaction Engineering
88713 SDC Green Challenge
88714 SDC Summer School in Unit Operations
88715 Biorefinery



# COURSES

## MSC, BSC, AND BENG COURSES

Below, course numbers and names are shown for 2017, 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.

**SPRING SEMESTER**

28012 Chemical and Biochemical Process Engineering (67) (B)
28016 Mathematical models for chemical and biochemical systems (61) (B)
28020 Introduction to Chemical and Biochemical Engineering (63)
28022 Unit Operations of Chemical Engineering and Biotechnology (56) (B)
28025 Bio Process Technology (70)
28121 Chemical Unit Operations Laboratory (7)
28122 Chemical Unit Operations Laboratory—3-week Summer University Laboratory (8)
28157 Process Design (45) (B)
28160 Mathematical models for chemical systems (32)
28212 Polymer Chemistry (40)
28214 Polymer Synthesis and Characterization (17)
28221 Chemical Engineering Thermodynamics (27)
28231 Laboratory in Chemical and Biochemical Engineering (25)
28271 Thermal gasification and sustainability (12)
28322 Chemical Engineering Thermodynamics (47) (B)
28342 Chemical Reaction Engineering (52) (B)
28344 Biotechnology and process design (38) (B)
28345 Chemical Reaction Engineering (31)
28346 Advanced fermentation technology practicum (5)
28350 Process Design: Principles and Methods (54)
28352 Chemical Process Control (59) (B)
28361 Chemical Engineering Model Analysis (48)
28415 Oil and Gas Production (25)
28423 Phase Equilibria for Separation Processes (10)
28434 Membrane Technology (44)
28443 Industrial Reaction Engineering (36)
28451 Optimizing Plantwide Control (17)
28811 Polymers in Processes and Products (10)
28850 Quality by Design (QbD): Integration of product and process development (73)
28855 Good Manufactoring Practice (56)
28864 Introduction to Matlab Programming (24)
28871 Production of Biofuels (30)
28885 Technology and Economy of Oil and Gas Production (22) (B)

**Courses offered in cooperation with other departments:**

12701 Introduction to Living systems (32)
26317 Instrumental Chemical Analysis (57)
41683 Materials Science (44) (B)

**FALL SEMESTER**

28001 Introduction to Chemistry and Chemical Engineering (70)
28012 Chemical and Biochemical Process Engineering (80) (B)
28016 Mathematical models for chemical and biochemical systems (49) (B)
28017 Chemical and Biochemical Process Engineering (22)
28022 Unit Operations of Chemical Engineering and Biotechnology (56) (B)
28121 Chemical Unit Operations Laboratory (28)
28125 Chemical Unit Operations Laboratory (21)
28140 Introduction to Chemical Reaction Engineering (50)
28150 Introduction to Process Control (63)
28157 Process and product design (38) (B)
28213 Polymer Technology (51)
28233 Recovery and Purification of Biological Products (68)
28242 Chemical Kinetics and Catalysis (69)
28244 Combustion and High Temperature Process (62)
28246 Applied Enzyme Technology and Kinetics (53)
28247 Advanced Enzyme Technology (13)
28310 Chemical and Biochemical Product Design (74)
28315 Colloid and Surface Chemistry (82)
28316 Laboratory Course in Colloid and Surface Chemistry (21)
28322 Chemical Engineering Thermodynamics (45) (B)
28342 Chemical Reaction Engineering (53) (B)
28344 Biotechnology and process design (43) (B)
28352 Chemical Process Control (43) (B)
28420 Separation Processes (55)
28515 Enhanced Oil Recovery (28)
28530 Transport Processes (49)
28831 Computational fluid dynamics in chemical engineering (20)
28845 Chemical Reaction Engineering Laboratory (21)
28852 Risk Assessment in Chemical Industry (74)
28864 Introduction to Matlab Programming (35)
28870 Energy and Sustainability (114)
28872 Biorefinery (42)

**Courses offered in cooperation with other departments:**

23522 Rheology of food and biological materials (14)
26010 Introductory Project in Chemistry (63)
27004 Health, Diseases and Technology (64)
41683 Materials Science (31) (B)

# BACHELOR OF ENGINEERING DEGREES

37 students finished their research programme for the BEng degree. The project titles and names of the students are listed below:

| | |
|---|---|
| **Abu-Eid, Sumer Ahmad Mohammad** | Wall deposition in spray dryers |
| **Akhtar, Raja Saadaqat Hamid** | TGA analysis of RDF particles |
| **Andersen, Rune Lundbeck** | Statistical model for optimal prediction of optimal pH for pectin extraction |
| **Balkiss, Mohammad** | Feed Pretreatment for Optimal Purification by Distillation |
| **Bjergholt, Christian** | Kinetics for Biomass Gasification |
| **Bjerring, Tobias Plæhn** | Biocatalytic synthesis of 5-Hydroxymethylfurfural to 2,5-diformylfuran |
| **Bodenhoff, Mia** | Investigation of a Possible Autocatalytic Effect in Catalytic Methanol Synthesis |
| **Elfang, Martin Kaufmann** | Mixing, Peeling and Polysaccharides |
| **Feldmann, Kevin Creutzberg** | Simulation, Design and Control of Internally Heat Integrated Distillation Columns |
| **Henriksen, Nikolaj Gersager** | Characterization of Pigment Particle Size and Rheology of Inkjet Inks |
| **Howarth, Leonora Juul** | Characterization of Coatings with Regards to Chemical Composition and Morphology |
| **Hussain, Javaid** | Conversion characteristics of RDF particles |
| **Jensen, Joachim Finn** | Optimization of a Membrane Characterization Model |
| **Jensen, Jonas Haugaard** | Investigation of Flocculation and Sedimentation of Brewer's Yeast |
| **Jørgensen, Lasse Ellegaard** | Model Based Monitoring of Column Separation Processes |
| **Kamp, Simon Kjær** | Production of Alkali from Cocoa Husk Ash for Extraction of Hydrocolloid from Biologically Pre-treated Brown Seaweed |
| **Larsen, Martin Rodenberg** | Experimental investigation of a cleaning in place ( CIP) pilot scale setup |
| **Marcher, Christina** | Investigation of the Possible Use of Surplus Heat from Nakskov Sugar Factory for District Heating |
| **Moustafa, Souhair** | Wall deposition in spray dryers |
| **Naimi, Semira** | Numerical Analysis of Differential Flow Instability in Packed Bed Reactors |
| **Navaneethan, Shagana** | Continuous MSMPR crystallization for pharmaceutical production |
| **Nielsen, Asger Egil Waagner** | Description of Polymer Film Deformation in the Stretch Hood Process |
| **Nielsen, Mette Stensgaard** | Experimental Determination of Operation Parameters for Enzyme Granulation with Glauber Salt |
| **Nielsen, Peter** | Experimental mixing time investigation of a large scale bio reactor |
| **Nørgreen, Andreas** | Selective fractionated crystallization of triglycerides |
| **Olsen, Anders Jul Stricker** | Studies on Trypsin Action on Insulin Substrates |
| **Pedersen, Mikkel** | Simulation Benchmark for Fermentation Processes |
| **Poulsen, Jesper Thor Funch** | Hydrophilic materials for the generation of the fourth phase of water |
| **Rasmussen, Søren Emil Høigaard** | Production of alkali from cocoa husk ash for extraction of hydrocolloid from biologically pretreated red seaweed |
| **Rimvall, Mikael Patrik** | Investigation of a Possible Autocatalytic Effect in Catalytic Methanol Synthesis |
| **Stigsby, Oliver Benjamin** | Optimization of arabinoxylan-extraction for biomaterials |
| **Strømsted, Astrid Kirsten** | Fluidized Bed Coating and Agglomeration |
| **Styrbæk, Peter** | Kinetics for Biomass Gasification |
| **Suliman, Kanar Khalid Ameen** | Modelling and Experimental Analysis of Cyclic Distillation |
| **Sørensen, Liv Lokia** | Description of the Kinetics for Catalytic Soot Oxidation |
| **Thaibesh, Ayah** | Investigation of the Importance of Attrition Resistance for the Physical Properties of Catalyst Pellets |
| **Topsøe, Frederik** | Hydrophilic materials for the generation of the fourth phase of water |

# BACHELOR OF SCIENCE DEGREES

25 students finished their research programme for the BSc degree. The project titles and names of the students are listed below:

| | |
|---|---|
| **Al-Azawi, Talal Khudhair Abbas** | Production of phosphoric acid from sludge, experimental and modeling study |
| **Andersen, Mads Lysgaard** | Catalytic hydrodeoxygenation of biomass pyrolysis oil model compounds |
| **Andersen, Thomas Guldbrand** | Study of Noble Metal Based $NH_3$ Oxidation Catalysts for Diesel Exhaust Aftertreatment |
| **Claudinger, Casper** | Preparation of tripple Janus particles |
| **Eriksen, Laurits Christoffer Skou** | Identification of an optimal bed material for a fluid bed process |
| **Hedegaard, Anna Kragh** | Development, Documentation and Demonstration of a Standardized Matlab-Simulink Model Implementation Procedure |
| **Jensen, Mikkel Munch** | Investigation of the formation of a heavy end during hydroprocessing of triglycerides |
| **Jørgensen, Emma Kathrine** | Catalytic conversion of lignin to value-added chemicals |
| **Jørsboe, Jens Kristian** | Measurement and Modelling of $CO_2$ Reaction Kinetics for Biogas Upgrading |
| **Krogsbøll, Laurits Bøggild** | High Pressure Pre-turbine SCR for $NO_x$ Reduction on Ships |
| **Lindahl, Simon Brædder** | Catalytic hydrodeoxygenation of biomass pyrolysis oil model compounds |
| **Lorits, Rune** | Combustion Chamber Development for Wood Stoves |
| **Mortensen, Michella Reimich** | Development of a Generic Plantwide Simulation Model for a Biotechnological Process |



## BACHELOR OF SCIENCE DEGREES

| | |
|---|---|
| **Møller, Andreas Christian** | Removal of cadmium from bio mass ash: Experiment and modeling |
| **Pedersen, Morten Lysdahlgaard** | Development of a Generic Plantwide Simulation Model for a Biotechnological Process |
| **Pham, Martin** | Solid-liquid equilibrium - data validation |
| **Rysgaard, Mathias Boe** | Oxidative leaching of chalcopyrite: Leaching dynamics and experimental constrains |
| **Rønsbro, Kristoffer** | Preparation and testing of FDCA based polyester thermosets |
| **Sandfeld, Camilla** | Preparation and Surface Functionalization of Magnetic Thiol-ene Particles |
| **Silau, Harald** | Surface modification of polysulfone membranes and immobilization of enzymes into these for biosynthetic membranes |
| **Stounberg, Jonathan** | Mapping of Tank Behavior Using CFD |
| **Sørensen, Philip Heldt** | Pilot-scale tests of catalytic cleaning technologies for diesel vehicles |
| **Sørensen, Thorbjørn Anker** | Modelling of energy losses in dielectric elastomer transducers |
| **Weis-Banke, Camilla Marie** | Synergy Studies of Mannan-degrading Enzymes |
| **Aagaard, Michel** | Characterisation of vanadium-based deNOx catalysts for automotive applications |

# MASTER OF SCIENCE DEGREES

70 students finished their research projects for the MSc degree. The project titles and names of the students are listed below:

| | |
|---|---|
| **Abdulrahman, Tareq** | Ignition of Biomass in Power Plant Mills |
| **Abouardini, Amin** | A Feasibility Study of Hydrocarbon Gas Injection in Skjold Field |
| **Al-Masri, Wael Fadi** | Carbon Dioxide Injection in North Sea Reservoirs |
| **Bennike, Rasmus Dziegiel** | Kinetic study of hydrodesulphurization and olefin saturation in FCC naphtha hydrotreating |
| **Berg, Casper Mølby** | A Feasibility Study of Hydrocarbon Gas Injection in Skjold Field |
| **Bülow, Mark** | Further Development and Investigations of the Electrolyte CPA Equation of State |
| **Cao, Yiyi** | Hybrid catalysts for combined removal of $NO_x$ and soot |
| **Duso, Alessandro** | Continuous MSMPR Crystallization Assisted by Gas Dispersion |
| **Eriksen, Gry Frost** | Characterisation of Continuous Fermentations of Saccharomyces Cerevisiae CEN.pk |
| **Fernandes Quilelli, Andres Eduardo** | Developing Quality Standards and Test Methods for the Rheological Characterization of a Non-Newtonian Slurry Suspension |
| **Foelsby, Jonas Richard** | Modeling of Flow and Heat Transport in Filament Stretching Rheometers |
| **Fraga Cabral Sacadura, Maria Do Carmo** | Food Waste upgrading by an Integrated Biorefinery Process |
| **Ghazvini, Mohammad Shabani** | Sulphation of Biomass Ash Deposits |
| **Glibstrup, Jens** | Numerical Fluid Dynamic Investigation of a Lactic Acid Bacteria Fermentation |
| **Grønborg, Jakob** | Preparation of PDMS block-copolymers for use as additives in coatings |
| **Haastrup, Erik** | Computational Fluid Dynamic Simulation and Experimental Investigation of a Static Mixer |
| **Hafthórsdóttir, Júlía Rós** | Numerical Investigation of the Fluid Dynamic Conditions in a Rotating Bed Reactor |
| **Hansen, Mads Hjælmsø** | Thermo-responsive Materials for Adhesives |
| **Hansen, Niklas Flink** | Thermodynamic Analysis of Oil Field Scale and Corrosion |
| **Hummelmose, Helene Kirstine** | Modelling of Catalyzed Diesel Particulate Filters for Combined Soot Removal and DeNOx |
| **Hybschmann, Tim Bylow** | Computational Fluid Dynamic (CFD) simulation of a rotational aeration system |
| **Jaksland, Anders** | Development of novel processing networks for biorefineries |
| **Jensen, Jacob Møller** | Superstructure based optimization of processing routes for $CO_2$ utilization |
| **Johannessen, Jeppe Charlie** | Deactivation of FeMo-Based Catalysts for Oxidation of Methanol to Formaldehyde |
| **Joshi, Parth Umesh** | MSMPR Crystallization for Continuous API Production |
| **Jørgensen, Anne-Marie Demuth** | Investigation of low temperature catalysts for ammonia synthesis |
| **Jørgensen, Luna Marie** | Frequency Content Analysis (FCA) Control as a Way to Detect and React to Metabolic Changes during Fermentations |
| **Karon, Hubert** | Temperature Dependency of Smart Waterflooding in Chalk |
| **Kennes Veiga, David Manuel** | Kinetics of Syngas' Fermentation to Methane and Ethanol |
| **Kirstrand, Rasmus Aslak Berlin** | Bacteriolytic Enzymes for Fuel Ethanol Control |
| **Klepczyk, Krystian Grzegorz** | Gas Re-Injection in North Sea Reservoirs |
| **Kolaczkowski, Bartlomiej** | Characterization of A-mannanases and Their Applications |
| **Kolaiti, Tereza** | Process design for the synthesis of biodiesel, glycerol, 3-hydroxypropionic acid and 1,3-propanediol |
| **Koumaditi, Evangelia** | Intensified Reaction-Separation Schemes |
| **Krum. Kristian Røhe Kongsted** | Decomposition of Urea |
| **Larsen, Julie Nør** | Design of a Sulfur Removal Unit for Biogas Upgrading Units |
| **Larsen, Michael Roland** | Simulation of Flow and Heat Transfer in Scanning Rheometer |
| **Lie, Erlend** | Optimisation of Tapping in Industrial Si-Production |
| **Lindeque, Rowan Malan** | P450 based Bioconversions |

## MASTER OF SCIENCE DEGREES

| | |
|---|---|
| **Lomsøy, Petter** | Experimental Determination of the Solubility of Scale Minerals at High Pressures and High Temperatures |
| **Meelby, Signe Katrine** | Reductive Activation of Chalcopyrite Particles |
| **Montet, Jean Etienne** | Effect of $Mg(OH)_2$ on Oxygen Delignification of Softwood Kraft Pulp |
| **Morfin, Alexis Pascal** | Synthesis of Polymers for Dual Curing Thermoset Systems |
| **Mortensen, Sara Refsgaard** | Hydrophilic Polyesters by Enzymatic Polymerization and their Application in Hydrogels as Enzyme Supports |
| **Nygaard, Christian Wolff** | Speciation of Phosphorus Chemistry in Ashes |
| **Pandey, Jyoti Shanker** | Environment- and Equipment-friendly Acidizing Fluid for Well Stimulation |
| **Papaspyrou, Christos** | Carbon Dioxide Injection in North Sea Reservoirs |
| **Portell Silva, Laura** | Systematic Optimization of Enzymatic Cellulose Saccharification of Lignocellulosic Biomass: Elephant Grass (Napier Grass), Sugarcane Bagasse, Sorghum Bagasse |
| **Price, Christian Sørensen** | Investigation of the Kinetics of Scale Formation |
| **Racanelli, Claudio** | Flowability of bulk solids |
| **Roien, Josephine Frederikke** | Impact of Morphological Development of Aspergillus Niger in Industrial Applications |
| **Santos Armajach, Gonzalo** | Synthesis of lactose based protein cross-linkers using enzyme cascades |
| **Saravia, Hugo Ignacio Mobarec** | Strict Anaerobic Fermentation |
| **Schandel, Christian Bækhøj** | Hydrogen assisted catalytic biomass pyrolysis for green fuels |
| **Seta, Olimpia** | Measurements and Correlation of PVT Properties for Biogas Upgrading $CO_2$ Removal Technologies |
| **Shukla, Ishan** | Modeling the Solubility of Exotic Scales at High Pressure and High Temperature |
| **Skjøtt, Monica Todorova Salari** | Optimising Heterologous VAR2 Protein Production in E. Coli |
| **Sobczyk, Pawl Konrad** | How to Use Linear and Non-Linear Rheology of Pressure Sensitive Adhesive for Ostomy Care |
| **Stilling, Torsten** | Thermodynamic Modelling and Heat Integration Simulation of $CO_2$ Compression and Liquefaction for EOR |
| **Subramanian Venkateswaran, Srinath** | Anticorrosive coatings at high temperatures and high pressures |
| **Tagliaferri, Stefano** | Surface Phenomena under Smart Waterflooding |
| **Tamaev, Nail** | Rheology Investigation of Antifouling Coatings for Improved Leveling |
| **Thanki, Mayur Kantilal** | Production and Economic Analysis of RJD Effect on Oil Recovery in the North Sea |
| **Theodorou, Panagiotis** | Evaluation of protein extraction protocols for macroalgae and plant biomass, and of the biomass degrading potential of unexploited microbial sources |
| **Thrane, Joachim** | Evaluation of protein extraction protocols for macroalgae and plant biomass, and of the biomass degrading potential of unexploited microbial sources |
| **Vercruyssen, Max** | Characterization of power efficiency in bioreactors |
| **Vik, Hedda Slatlem** | A Coupled THM Simulation for Fractured Reservoirs |
| **Wang, Ting** | Diffusion of Acids in Protective Organic Coatings |
| **Wright, Mathias Risager** | Numerical simulations of fluid dynamic conditions in a large scale fermentation vessel including the effect of kinetic growth models for the microorganism |
| **Wybraniec, Ewa Agnieszka** | Study of enzymatic conversion of peptide hormone |

## SDC MASTER DEGREES

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

| | |
|---|---|
| **Cheng, Yonggang** | Exothermic heat transfer in syngas methanation in transport bed reactor |
| **Fan, Haonan** | Antibiotic resistance genes and its association with bacterial Communities during vacuum-type aerobic manure composting |
| **Fang, Xiaowei** | Synthesis of 5-hydroxymethylfurfural (HMF) from cellulose |
| **Gao, Kai** | Direct conversion of cellulose into sorbitol by ionic liquids |
| **Hu, Pengpeng** | Selective leaching of lithium and gallium from high aluminum coal fly ash |
| **Li, Weijun** | Multi-objective modeling and optimization of biogas system |
| **Li, Xiankai** | The wrinkles in graphene induced by supercontration of spider silk and their applications in flexible sensors |
| **Lv, Dong** | Preparation and Characterization of Cellulose Nanofibrils |
| **Ma, Congkai** | Synthesis of Polycarbonate from isosorbide and DMC Catalyzed by Ionic Liquids |
| **Ma, Nicolai** | Enzyme immobilization on ceramic membranes |
| **Niu, Yan** | DDPM Simulation of MTO fluidized bed reactor |
| **Su, Ziran** | Production of Oligodextran with Uniform Molecular Weight by using Enzymatic Membrane Reactor |
| **Wu, Xiao** | Synthesis of mussel-inspired polyvinylpyrrolidone based adhesive for underwater bonding |
| **Zhao, Tong** | DFT study for the mechanism of char-NO heterogeneous reaction |
| **Zhang, Jianfeng** | Extration and separation of rubidium and cesium from salt lake |
| **Zhang, Yingying** | Novel Synthetic methodology for Epoxidized Natural Rubber and Optimation of Damping Property |



A spray nozzle is used to generate droplets in oil burners. Here is a nozzle operated with water so that measurements of the droplet properties can be conducted.

Photo: Thorkild Christensen

# THE FACULTY **2017**

**SCIENTIFIC**


Jens Abildskov
Associate Professor


Jakob Munkholt Christensen
Assistant Professor


Kim Dam-Johansen
Professor,
Head of Dept.


Anders Egede Daugaard
Associate Professor


Philip Fosbøll
Associate Professor


Rafiqul Gani
Professor


Hariklia N. Gavala
Associate Professor


Krist V. B. Gernaey
Professor


Peter Glarborg
Professor


Ole Hassager
Professor


Jakob Kjøbsted Huusom
Associate Professor


Martin Høj
Assistant Professor


Anker D. Jensen
Professor


Søren Kiil
Associate Professor


Georgios M. Kontogeorgis
Professor


Ulrich Krühne
Associate Professor


Xiaodong Liang
Assistant Professor


Anne S. Meyer
Professor


Anna E. Lantz
Associate Professor


Manuel Pinelo
Associate Professor


Alexander A. Shapiro
Associate Professor


Gürkan Sin
Associate Professor


Ioannis V. Skiadas
Associate Professor


Anne Ladegaard Skov
Associate Professor


Nicolas von Solms
Associate Professor


Peter Szabo
Associate Professor


Kaj Thomsen
Associate Professor

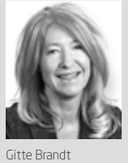

Stig Wedel
Associate Professor


John Woodley
Professor


Hao Wu
Assistant Professor


Hanne Østergård
Research Specialist

**ADMINISTRATIVE AND OPERATIVE**


Gitte Brandt
Head of Secretariat


Ivan Hundebøl
Special Consultant,
PILOT PLANT


Steen Larsen
Head of PILOT PLANT

**EMERITUS**


Gunnar Jonsson
Associate Professor
Emeritus


Sten Bay Jørgensen
Professor Emeritus


Michael L. Michelsen
Professor Emeritus
(Docent)


John Villadsen
Professor Emeritus


Lars G. Kiørboe
Emeritus


Karsten H. Clement
Professor Emeritus



# KTSTUDENTS



Our student organization, KTStudents, represents all students in the courses at the department. Its goal is to improve the study environment for students through social and professional activities.

< From left to right: Adem Rosenkvist, Beatrice Mazzali, Monica Abildgaard, Mathias Johansen, Jeska Naujoks, and Akhilesh Nair.
Photo: Christian Ove Carlsson

### Company presentations

Companies within the chemical and biochemical areas are invited to present their daily work and challenges. The company presentations give the students a better understanding of their potential future jobs, an opportunity to network and thereby a way for the students to attain projects, internships, or student jobs.

### Company visits

The students are given the opportunity to visit companies within the chemical and biochemical fields. The tours around the production plants give the students insight into large-scale industry and the surrounding working environment.

### Social events

Through social events, students get to socialize and network with other students. These activities especially strengthen the network between international and Danish students.

### Liaison between the department and the students

In addition to providing knowledge about what a career in the chemical engineering industry entails, KTStudents also aims to help the academic development of chemical engineering students by acting as a liaison between the department and the students. We aim to expose students to research undertaken at DTU Chemical Engineering to generate awareness about the research centres and to facilitate a direction for BSc, MSc, or PhD thesis topics.

# GUESTS

## VISITING PHD STUDENTS

**Alessandro Rosengart** from Politecnico di Milano, Italy
**Alistar Rodman** from University of Edinburgh, Scotland
**Asma Rafsanjani** from University of Tehran, Iran
**Ayse Dilan Celebi** from EPFL, Switzerland
**Chen Hailin** from University of Chinese Academy of Sciences, China
**Chen Lyu** from China University of Mining and Technology (Beijing), China
**Daniela Damaceno** from University of Compinas, Brazil
**Daniela Valencia Sánchez** from Universitat Autònoma de Barcelona, Spain
**Dasom Im** from KAIST, South Korea
**Dingrong Kang** from University of Copenhagen, Denmark
**Dmitrii Denishchuk** from MPEI Institute, Russia
**Dong Chen** from RCEES, Chinese Academy of Science, China
**Donglin Xin** from Northwese University, China
**Edward Acheampong** from University of Nottingham, United Kingdom
**Eirin Abrahamsen** from University of Stavanger, Norway
**Ghochapon Mongkhonsiri** from Chulalongkorn University, Thailand
**Johannes Ami** from KNUST, Ghana
**Kai Kang** from Xi'an Jiaotong University, China
**Kamil Dino Adem** from Addis Ababa University, Ethiopia
**Maryam Huseini** from Tarbiat Modares University, Iran
**Matej Danko** from Slovak University of Technology in Bratislava, Slovakia
**Mattia Turchi** from Unilever UK, United Kingdom
**Oluwatosin Fabusuyi** from University of Lisbon, Portugal
**Rafael Tini** from Universidade do Estado do Rio de Janeiro, Brazil
**Samira Mohammadkhani** from Isfahan University of Technology, Iran
**Sehouah Mouhoubi** from University of Mons, Belgium
**Shaoqi Yang** from IPE, Chinese Academy of Science, China
**Shaorui Zhang** from Zhejiang University, China
**Song Xu** from IPE, Chinese Academy of Science, China
**Tianyuan Wang** from PSL Research University, France
**Viktor Konakovsky** from Newcastle University, United Kingdom
**Xinsheng Hu** from China University of Mining and Technology (Beijing), China
**Zhongfa Hu** from Xian Jiaotong University, China

## OTHER VISITORS

**Postdoc Adrian Bele** from Petru Poni Institute of Macromolecular Chemistry, Romania
**Postdoc Hongliang Qian** from China Pharmaceutical University, China
**Postdoc Piyapong Hunpinyo** from King Mongkut's University of Technology, Thailand
**Postdoc Teng Zhou** from Max Planck Institute, Germany
**Dr. Jisong Bai** from Chongqing University of Science & Technology, China
**Associate Professor Haifeng Dong** from IPE, Chinese Academy of Science, China
**Associate Professor Ivonne Garcia Rodriguez** from Institut National Polytechnique de Toulouse, France
**Associate Professor Oskar Karlström** from Åbo Universitet, Finland
**Associate Professor Xuguang Tang** from IPE, Chinese Academy of Science, China
**Associate Professor Zhimim Lu** from South China University of Technology, China
**Professor Dimitris Vlassopoulos** from University of Crete, Greece
**Professor Junwu Wang** from IPE, Chinese Academy of Science, China
**Professor Michael Brook** from McMaster University, Canada
**Professor Min Liu** from University of Science and Technology, China
**Professor Ramsagar Vooradi** from NIT, India
**Professor Roald Kaommedal** from University of Stavanger, Norway
**Professor Sarath Babu Anne** from NIT, India
**Professor Xiuhong Yang** from IPE, Chinese Academy of Science, China
**Professor Zhenyu Tian** from Chinese Academy of Sciences, China

# PUBLICATIONS

**Process Development for Biocatalysis**
Oxidation of macrocyclic ketones to lactones catalyzed by a Baeyer–Villiger monooxygenase (BVMO), an oxygen-dependent enzyme.

Photo: Thorkild Christensen

## WoS publications

A Razak, Aliff Hisyam; Skov, Anne Ladegaard / **Silicone elastomers with covalently incorporated aromatic voltage stabilisers.** RSC Advances, Vol. 7, No. 1, 2017, pp. 468-477.

A Razak, Aliff Hisyam; Yu, Liyun; Skov, Anne Ladegaard / **Voltage-stabilised elastomers with increased relative permittivity and high electrical breakdown strength by means of phase separating binary copolymer blends of silicone elastomers.** R S C Advances, Vol. 7, 2017, pp. 17848-17856.

Anantasarn, Nateetorn; Suriyapraphadilok, Uthaiporn; Babi, Deenesh Kavi / **A computer-aided approach for achieving sustainable process design by process intensification.** Computers and Chemical Engineering, Vol. 105, 2017, pp. 56-73.

Andersen, Nina Marianne; Cognet, T.; Santacoloma, P. A.; Larsen, J.; Armagan, I.; Larsen, F. H.; Gernaey, Krist; Abildskov, Jens; Huusom, Jakob Kjøbsted / **Dynamic modelling of pectin extraction describing yield and functional characteristics.** Journal of Food Engineering, Vol. 192, 2017, pp. 61-71.

Arora, S.; Shabbir, A.; Hassager, O.; Ligoure, C.; Ramos, L. / **Brittle fracture of polymer transient networks.** Journal of Rheology, Vol. 61, No. 6, 2017, pp. 1267-1275.

Arrad, Mouad; Kaddami, Mohammed; El Goundali, Bahija; Thomsen, Kaj / **Solubility modeling of the systems $Ni(NO_3)_2$-$H_2O$ and $Fe(NO_3)_3$-$Ni(NO_3)_2$-$H_2O$ with the extended universal quasichemical (UNIQUAC) model.** Journal of Solution Chemistry, Vol. 46, No. 6, 2017, pp. 1220-1229.

Arya, Alay; Liang, Xiaodong; von Solms, Nicolas; Kontogeorgis, Georgios / **Modeling of asphaltene precipitation from crude oil with the cubic plus association equation of state.** Energy and Fuels, Vol. 31, No. 2, 2017, pp. 2063-2075.

Arya, Alay; Liang, Xiaodong; von Solms, Nicolas; Kontogeorgis, Georgios / **Prediction of gas injection effect on asphaltene precipitation onset using the cubic and cubic-plus-association equations of state.** Energy and Fuels, Vol. 31, No. 3, 2017, pp. 3313-3328.

Bach, Christian; Yang, Jifeng; Larsson, Hilde Kristina; Stocks, Stuart M.; Gernaey, Krist; Albæk, Mads Orla; Krühne, Ulrich / **Evaluation of mixing and mass transfer in a stirred pilot scale bioreactor utilizing CFD.** Chemical Engineering Science, Vol. 171, 2017, pp. 19-26.

Banik, Sindrila Dutta; Nordblad, Mathias; Woodley, John M.; Peters, Günther H.J. / **Effect of water clustering on the activity of Candida antarctica lipase B in organic medium.** Catalysts, Vol. 7, No. 8, 227, 2017.

Baroi, G. N.; Gavala, Hariklia N.; Westermann, P.; Skiadas, Ioannis / **Fermentative production of butyric acid from wheat straw: Economic evaluation.** Industrial Crops and Products, Vol. 104, 2017, pp. 68-80.

Barton, Emma J.; Yurchenko, Sergei N.; Tennyson, Jonathan; Clausen, Sønnik; Fateev, Alexander / **High-resolution absorption measurements of $NH_3$ at high temperatures: 2100-5500 $cm^{-1}$.** Journal of Quantitative Spectroscopy & Radiative Transfer, Vol. 189, 2017, pp. 60-65.

Battini, Fabio; Grønlund, Mette; Agnolucci, Monica; Giovannetti, Manuela; Jakobsen, Iver / **Facilitation of phosphorus uptake in maize plants by mycorrhizosphere bacteria.** Scientific Reports, Vol. 7, No. 1, 4686, 2017.

Baum, Andreas; Dominiak, Malgorzata Maria; Vidal-Melgosa, Silvia; Willats, William G. T.; Søndergaard, Karen M.; Hansen, Per W.; Meyer, Anne S.; Mikkelsen, Jørn Dalgaard / **Prediction of pectin yield and quality by FTIR and carbohydrate microarray analysis.** Food and Bioprocess Technology, Vol. 10, No. 1, 2017, pp. 143-154.

Bertran, Maria-Ona; Frauzem, Rebecca; Sanchez-Arcilla, Ana Sofia; Zhang, Lei; Woodley, John; Gani, Rafiqul / **A generic methodology for processing route synthesis and design based on superstructure optimization.** Computers and Chemical Engineering, Vol. 106, 2017, pp. 892-910.

Binti Jamek, Shariza; Nyffenegger, Christian; Muschiol, Jan; Holck, Jesper; Meyer, Anne S.; Mikkelsen, Jørn Dalgaard / **Characterization of two novel bacterial type A exo-chitobiose hydrolases having C-terminal 5/12-type carbohydrate-binding modules.** Applied Microbiology and Biotechnology, Vol. 101, No. 11, 2017, pp. 4533-4546.

Bisgaard, Thomas; Mauricio Iglesias, Miguel; Huusom, Jakob Kjøbsted; Gernaey, Krist V.; Dohrup, Jesper; Petersen, Mikael A.; Abildskov, Jens / **Adding value to bioethanol through a purification process revamp.** Industrial and Engineering Chemistry Research, Vol. 56, No. 19, 2017, pp. 5692-5704.

Bisgaard, Thomas; Skogestad, Sigurd; Abildskov, Jens; Huusom, Jakob Kjøbsted / **Optimal operation and stabilising control of the concentric heat-integrated distillation column (HIDiC).** Computers & Chemical Engineering, Vol. 96, 2017, pp. 196-211.

Boiocchi, Riccardo; Gernaey, Krist; Sin, Gürkan / **A novel fuzzy-logic control strategy minimizing $N_2O$ emissions.** Water Research, Vol. 123, 2017, pp. 479-494.

Boiocchi, Riccardo; Gernaey, Krist; Sin, Gürkan / **Understanding $N_2O$ formation mechanisms through sensitivity analyses using a plant-wide benchmark simulation model.** Chemical Engineering Journal, Vol. 317, 2017, pp. 935-951.

Bruhn, Annette; Janicek, Tina; Manns, Dirk Martin; Nielsen, Mette Møller; Balsby, Thorsten Johannes Skovbjerg; Meyer, Anne S.; Rasmussen, Michael Bo; Hou, Xiaoru; Saake, Bodo; Göke, Cordula; Bjerre, Anne-Belinda / **Crude fucoidan content in two North Atlantic kelp species, Saccharina latissima and Laminaria digitata - seasonal variation and impact of environmental factors.** Journal of Applied Phycology, Vol. 29, No. 6, 2017, pp. 3121-3127.

Busk, Peter Kamp; Pilgaard, Bo; Lezyk, Mateusz Jakub; Meyer, Anne S.; Lange, Lene / **Homology to peptide pattern for annotation of carbohydrate-active enzymes and prediction of function.** B M C Bioinformatics, Vol. 18, 214, 2017.

Capellades Mendez, Gerard; Kiil, Søren; Dam-Johansen, Kim; Mealy, Michael J.; Christensen, Troels V. ; Myerson, Allan S. / **Effect of air injection on nucleation rates : An approach from induction time statistics.** Crystal Growth & Design, Vol. 17, No. 6, 2017, pp. 3287-3294.

Carolina Figueroa Murcia, Diana; Fosbøl, Philip Loldrup; Thomsen, Kaj; Stenby, Erling Halfdan / **Determination of zinc sulfide solubility to high temperatures.** Journal of Solution Chemistry, Vol. 46, No. 9-10, 2017, pp. 1805-1817.

Cernuschi, Federico; Rothleitner, Christian; Clausen, Sønnik; Neuschaefer-Rube, Ulrich; Illemann, Jens; Lorenzoni, Lorenzo; Guardamagna, Cristina; Larsen, Henning Engelbrecht / **Accurate particle speed prediction by improved particle speed measurement and 3-dimensional particle size and shape characterization technique.** Powder Technology, Vol. 318, 2017, pp. 95-109.

Chakraborty , Debasish; Damsgaard, Christian Danvad; Silva, Hugo José Lopes; Conradsen, Christian Nagstrup; Olsen, Jakob Lind; de Carvalho, Hudson W. P.; Mutz, Benjamin; Bligaard, Thomas ; Hoffmann, Max J; Grunwaldt, Jan-Dierk; Studt, Felix; Chorkendorff, Ib / **Bottom-up design of a copper-ruthenium nanoparticulate catalyst for low-temperature ammonia oxidation.** Angewandte Chemie (International Edition), Vol. 56, No. 30, 2017, pp. 8711-8715.

Choudhury, H. A.; Intikhab, S.; Kalakul, Sawitree; Khan, Muhammad Salman; Tafreshi, R.; Gani, Rafiqul; Elbashir, N. O. / **Designing a surrogate fuel for gas-to-liquid derived diesel.** Energy and Fuels, Vol. 31, No. 10, 2017, pp. 11266-11279.

Christensen, Jakob Munkholt; Grunwaldt, Jan-Dierk; Jensen, Anker Degn / **Effect of $NO_2$ and water on the catalytic oxidation of soot.** Applied Catalysis B: Environmental, Vol. 205, 2017, pp. 182-188.

Chung, Wing Sun Faith; Meijerink, Marjolein; Zeuner, Birgitte; Holck, Jesper; Louis, Petra; Meyer, Anne S.; Wells, Jerry M; Flint, Harry J; Duncan, Sylvia H / **Prebiotic potential of pectin and pectic oligosaccharides to promote anti-inflammatory commensal bacteria in the human colon.** Fems Microbiology Ecology, Vol. 93, No. 11, fix127, 2017.

Cignitti, Stefano; Andreasen, Jesper Graa; Haglind, Fredrik; Woodley, John; Abildskov, Jens / **Integrated working fluid-thermodynamic cycle design of organic Rankine cycle power systems for waste heat recovery.** Applied Energy, Vol. 203, 2017, pp. 442-453.

Damø, Anne Juul; Jensen, Peter Arendt; Jappe Frandsen, Flemming; Wu, Hao; Glarborg, Peter / **Fly ash formation during suspension-firing of biomass. Effects of residence time and fuel-type.** Energy & Fuels, Vol. 31, No. 1, 2017, pp. 555-570.

de Hemptinne, J.-C; Ferrasse, J.-H.; Górak, A.; Kjelstrup, S.; Marechal, F.; Baudouin, O.; Gani, Rafiqul / **Energy efficiency as an example of cross-discipline collaboration in chemical engineering.** Chemical Engineering Research and Design, Vol. 119, 2017, pp. 183-187.

Domingo-Felez, Carlos; Calderó-Pascual, María; Sin, Gürkan; Plósz, Benedek G.; Smets, Barth F. / **Calibration of the comprehensive NDHA-$N_2O$ dynamics model for nitrifier-enriched biomass using targeted respirometric assays.** Water Research, Vol. 126, 2017, pp. 29-39.

Dotsenko, Gleb; Lange, Lene / **Enzyme enhanced protein recovery from green biomass pulp.** Waste and Biomass Valorization, Vol. 8, No. 4, 2017, pp. 1257-1264.

Duan, Yun Feng; Reinsch, Sabine; Ambus, Per; Elsgaard, Lars; Petersen, Søren O. / **Activity of type i methanotrophs dominates under high methane concentration: Methanotrophic activity in slurry surface crusts as influenced by methane, oxygen, and inorganic nitrogen.** Journal of Environmental Quality, Vol. 46, No. 4, 2017, pp. 767-775.

Duhn, Jakob Dragsbæk; Jensen, Anker Degn; Wedel, Stig; Wix, Christian / **Modeling of gas diffusion in Ni/YSZ electrodes in $CO_2$ and Co-electrolysis.** Fuel Cells, Vol. 17, No. 4, 2017, pp. 442-456.

Eftekhari, Ali Akbar; Thomsen, Kaj; Stenby, Erling Halfdan; Nick, Hamidreza M. / **Thermodynamic analysis of chalk-brine-oil interactions.** Energy and Fuels, Vol. 31, No. 11, 2017, pp. 11773-11782.

Elliot, Samuel Gilbert; Andersen, Christian; Tolborg, Søren; Meier, Sebastian; Sadaba, I. ; Daugaard, Anders Egede; Taarning, E. / **Synthesis of a novel polyester building block from pentoses by tin-containing silicates.** RSC Advances, Vol. 7, 2017, pp. 985-996.

Feldman, Hannah; Flores Alsina, Xavier; Ramin, Pedram; Kjellberg, K.; Jeppsson, U.; Batstone, Damien J.; Gernaey, Krist V. / **Modelling an industrial anaerobic granular reactor using a multi-scale approach.** Water Research, Vol. 126, 2017, pp. 488-500.

Feng, Kai; Zhang, Zhaojing; Cai, Weiwei; Liu, Wenzong; Xu, Meiying; Yin, Huaqun; Wang, Aijie; He, Zhili; Deng, Ye / **Biodiversity and species competition regulate the resilience of microbial biofilm community.** Molecular Ecology, Vol. 26, No. 21, 2017, pp. 6170-6182.

Frankær, Christian Grundahl; Sønderby, Pernille; Bang, Maria Blanner; Mateiu, Ramona Valentina; Groenning, Minna; Bukrinski, Jens; Harris, Pernille / **Insulin fibrillation: The influence and coordination of $Zn^{2+}$.** Journal of Structural Biology, Vol. 199, No. 1, 2017, pp. 27-38.

Frutiger, Jerome; Bell, Ian; O'Connell, John P.; Kroenlein, Kenneth; Abildskov, Jens; Sin, Gürkan / **Uncertainty assessment of equations of state with application to an organic Rankine cycle.** Molecular Physics, Vol. 115, No. 9-12, 2017, pp 1235-1244.

Fu, Zhaolin; Wang, Z.; Lin, Weigang; Song, Wenli / **Conversion of furan derivatives for preparation of biofuels over Ni-Cu/C catalyst.** Energy Sources. Part A. Recovery, Utilization, and Environmental Effects, Vol. 39, No. 11, 2017, pp. 1176-1181.

Fu, Zhaolin; Wang, Ze; Lin, Weigang; Song, Wenli; Li, Songgeng / **High efficient conversion of furfural to 2-methylfuran over Ni-Cu/$Al_2O_3$ catalyst with formic acid as a hydrogen donor.** Applied Catalysis A: General, Vol. 547, 2017, pp. 248-255.

Gadsbøll, Rasmus Østergaard; Thomsen, Jesper; Bang-Møller, Christian; Ahrenfeldt, Jesper; Henriksen, Ulrik Birk / **Solid oxide fuel cells powered by biomass gasification for high efficiency power generation.** Energy, Vol. 131, 2017, pp. 198-206.

Gani, Rafiq / **Editorial - In honor of Professor Rafiqul Gani.** Computers and Chemical Engineering, Vol. 107, 2017, pp. 1-2.

Gaspar, Jozsef; Fosbøl, Philip Loldrup / **Practical enhancement factor model based on GM for multiple parallel reactions: Piperazine (PZ) $CO_2$ capture.** Chemical Engineering Science, Vol. 158, 2017, pp. 257-266.

Gersen, Sander; van Essen, Martijn; Darmeveil, Harry; Hashemi, Hamid; Rasmussen, Christian Tihic; Christensen, Jakob Munkholt; Glarborg, Peter; Levinsky, Howard / **Experimental and modeling investigation of the effect of $H_2S$ addition to methane on the ignition and oxidation at high pressures.** Energy & Fuels, Vol. 31, No. 3, 2017, pp. 2175-2182.

Gladis, Arne; Deslauriers, Maria Gundersen; Fosbøl, Philip Loldrup; Woodley, John; von Solms, Nicolas / **Influence of temperature and solvent concentration on the kinetics of the enzyme carbonic anhydrase in carbon capture technology.** Biochemical Engineering Journal, Vol. 309, 2017, pp. 772-786.

Glarborg, Peter; Marshall, Paul / **Importance of the hydrogen isocyanide isomer in modeling hydrogen cyanide oxidation in combustion.** Energy & Fuels, Vol. 31, No. 3, 2017, pp. 2156-2163.

Gracia-Lor, Emma; Rousis, Nikolaos I.; Zuccato, Ettore; Bade, Richard; Baz-Lomba, Jose Antonio; Castrignanò, Erika; Causanilles Llanes, Ana; Hernández, Félix; Kasprzyk-Hordern, Barbara; Kinyua, Juliet; McCall, Ann-Kathrin; van Nuijs, Alexander L. N.; Plósz, Benedek G.; Ramin, Pedram; Ryu, Yeonsuk; Santos, Miguel M.; Thomas, Kevin V.; de Voogt, Pim; Yang, Zhugen; Castiglioni, Sara / **Estimation of caffeine intake from analysis of caffeine metabolites in wastewater.** Science of the Total Environment, Vol. 609, 2017, pp. 1582-1588.

Haddad, Nizar Jamal; Al-Nakeeb, Kosai Ali Ahmed; Petersen, Bent; Dalén, Love; Sorgenfrei Blom, Nikolaj; Sicheritz-Pontén, Thomas / **Complete mitochondrial genome of the Oriental Hornet, Vespa orientalis F. (Hymenoptera: Vespidae).** Mitochondrial DNA Part B, Vol. 2, No. 1, 2017, pp. 139-140.

Halim, Amalia Yunita; Nielsen, Sidsel Marie; Nielsen, Kristian Fog; Eliasson Lantz, Anna / **Towards the understanding of microbial metabolism in relation to microbial enhanced oil recovery.** Journal of Petroleum Science and Engineering, Vol. 149, 2017, pp. 151-160.

Hansen, Stine Broholm; Jensen, Peter Arendt; Jappe Frandsen, Flemming; Sander, Bo; Glarborg, Peter / **Mechanistic model for ash deposit formation in biomass suspension firing. Part 1: Model verification by use of entrained flow reactor experiments.** Energy and Fuels, Vol. 31, No. 3, 2017, pp. 2771–2789.

Hansen, Stine Broholm; Jensen, Peter Arendt; Jappe Frandsen, Flemming; Sander, Bo; Glarborg, Peter / **Mechanistic model for ash deposit formation in biomass suspension-fired boilers. Part 2: Model verification by use of full scale tests.** Energy and Fuels, Vol. 31, No. 3, 2017, pp. 2790-2802.

Hansen, Thomas Klint; Høj, Martin; Hansen, Brian Brun; Janssens, Ton V.W.; Jensen, Anker Degn / **The effect of pt particle size on the oxidation of CO, $C_3H_6$, and NO over $Pt/Al_2O_3$ for diesel exhaust aftertreatment.** Topics in Catalysis, Vol. 60, No. 17-18, 2017, pp. 1333-1344.

Hashemi, Hamid; G. Jacobsen, Jon ; Rasmussen, Christian T. ; Christensen, Jakob Munkholt; Glarborg, Peter; Gersen, Sander; van Essen, Martijn; B. Levinsky, Howard ; Klippenstein, Stephen J. / **High-pressure oxidation of ethane.** Combustion and Flame, Vol. 182, 2017, pp. 150-166.

Hassouneh, Suzan Sager; Yu, Liyun; Skov, Anne Ladegaard; Daugaard, Anders Egede / **Soft and flexible conductive PDMS/MWCNT composites.** Journal of Applied Polymer Science, Vol. 134, No. 18, 44767, 2017.

Heintz, Søren; Börner, Tim; Ringborg, Rolf Hoffmeyer; Rehn, Gustav; Grey, Carl; Nordblad, Mathias; Krühne, Ulrich; Gernaey, Krist; Adlercreutz, Patrick; Woodley, John / **Development of in-situ product removal strategies in biocatalysis applying scaled-down unit operations.** Biotechnology and Bioengineering, Vol. 114, No. 3, 2017, pp. 600-609.

Hoffmann, Christian; Pinelo, Manuel; Woodley, John; Daugaard, Anders Egede / **Development of a thiol-ene based screening platform for enzyme immobilization demonstrated using horseradish peroxidase.** Biotechnology Progress, Vol. 33, No. 5, 2017, pp. 1267-1277.

Hoffmann, Christian; Pereira Rosinha Grundtvig, Ines; Thrane, Joachim; Garg, Nipun; Gernaey, Krist V.; Pinelo, Manuel; Woodley, John; Krühne, Ulrich; Daugaard, Anders Egede / **Experimental and computational evaluation of area selectively immobilized horseradish peroxidase in a microfluidic device.** Chemical Engineering Journal, Vol. 332, 2017, pp. 16-23.

Huang, Qian; Costanzo, S.; Das, C.; Vlassopoulos, Dimitrios / **Stress growth and relaxation of dendritically branched macromolecules in shear and uniaxial extension.** Journal of Rheology, Vol. 61, No. 1, 2017, pp. 35-47.

Huang, Qian; Hassager, Ole / **Polymer liquids fracture like solids.** Soft Matter, Vol. 13, 2017, pp. 3470-3474.

Huang, Qian; Rasmussen, Henrik K. / **The transition between undiluted and oligomer-diluted states of nearly monodisperse polystyrenes in extensional flow.** Rheologica Acta, Vol. 56, No. 9, 2017, pp. 719-727.

Javakhishvili, Irakli; Dimitrov, Ivaylo; Tynelius, Oskar; Hales, Jan Harry; Jankova Atanasova, Katja ; Hvilsted, Søren / **Surface-initiated atom transfer radical polymerization from electrospun mats: An alternative to Nafion.** Macromolecular Materials & Engineering, Vol. 302, No. 4, 1600410, 2017.

Jers, Carsten; Strube, Mikael Lenz; Cantor, Mette D; Nielsen, Bea K K; Sørensen, Ole Brøsted; Boye, Mette; Meyer, Anne S. / **Selection of Bacillus species for targeted in situ release of prebiotic galacto-rhamnogalacturonan from potato pulp in piglets.** Applied Microbiology and Biotechnology, Vol. 101, No. 9, 2017, pp. 3605-3615.

Jørgensen, Henning; Pinelo, Manuel / **Enzyme recycling in lignocellulosic biorefineries.** Biofuels, Bioproducts and Biorefining, Vol. 11, 2017, pp. 150-167.

Kalafatakis, Stavros; Braekevelt, Sylvie; Carlsen, Vilhelmsen; Lange, Lene; Skiadas, Ioannis V.; Gavala, Hariklia N. / **On a novel strategy for water recovery and recirculation in biorefineries through application of forward osmosis membranes.** Chemical Engineering Journal, Vol. 311, 2017, pp. 209-216.

Karcz, Adam Paul; Damø, Anne Juul; Illerup, Jytte Boll; Rocks, Sara; Dam-Johansen, Kim; Chaiko, David / **Electron microscope investigations of activated chalcopyrite particles via the FLSmidth® ROL process.** Journal of Materials Science, Vol. 52, No. 20, 2017, pp. 12044-12053.

Khakimov, Bekzod; Christiansen, Lene D.; Heins, Anna-Lena; Sørensen, Klavs M.; Schöller, Charlotte Elisabeth Grüner; Clausen, Anders; Skov, Thomas; Gernaey, Krist V.; Engelsen, Søren B. / **Untargeted GC-MS metabolomics reveals changes in the metabolite dynamics of industrial scale batch fermentations of streptoccoccus thermophilus broth.** Biotechnology Journal, Vol. 12, 1700400, 2017.

Kiil, Søren / **Mathematical modeling of pigment dispersion taking into account the full agglomerate particle size distribution.** Journal of Coatings Technology and Research, Vol. 14, No. 1, 2017, pp. 69-84.

Kourmentza, Constantina; Plácido, Jersson; Venetsaneas, Nikolaos; Burniol Figols, Anna; Varrone, Cristiano; Gavala, Hariklia N.; Rei, Maria A. M. / **Recent advances and challenges towards sustainable polyhydroxyalkanoate (PHA) production.** Journal of Bioscience and Bioengineering, Vol. 4, No. 2, 55, 2017.

Kumar Tula, Anjan; Babi, Deenesh K.; Bottlaender, Jack; Eden, Mario R.; Gani, Rafiqul / **A computer-aided software-tool for sustainable process synthesis-intensification.** Computers and Chemical Engineering, Vol. 105, 2017, pp. 74-95.

Larsson, Hilde Kristina; Schjøtt Andersen, Patrick Alexander; Byström, Emil; Gernaey, Krist; Krühne, Ulrich / **CFD modeling of flow and ion exchange kinetics in a rotating bed reactor system.** Industrial & Engineering Chemistry Research, Vol. 56, No. 14, 2017, pp. 3853-3865.

Laxminarayan, Yashasvi; Jensen, Peter Arendt; Wu, Hao; Jappe Frandsen, Flemming; Sander, Bo; Glarborg, Peter / **Deposit shedding in biomass-fired boilers: Shear adhesion strength measurements.** Energy and Fuels, Vol. 31, No. 8, 2017, pp. 8733-8741.

Le, Duy Michael; Damgaard Nielsen, Anders; Sørensen, Hanne; Meyer, Anne S. / **Characterisation of authentic lignin biorefinery samples by Fourier transform infrared spectroscopy and determination of the chemical formula for lignin.** Bioenergy Research, Vol. 10, No. 4, 2017, pp. 1025-1035.

Le, Duy Michael; Sorensen, Hanne R.; Meyer, Anne S. / **Elemental analysis of various biomass solid fractions in biorefineries by X-ray fluorescence spectrometry.** Biomass and Bioenergy, Vol. 97, 2017, pp. 70-76.

Le, Duy Michael; Sorensen, Hanne R.; Meyer, Anne S. / **Pre-process desilication of wheat straw with citrate.** Process Biochemistry, Vol. 55, 2017, pp. 126-132.

Liang, Xiaodong; Aloupis, Georgios; Kontogeorgis, Georgios M. / **Data requirements and modeling for gas hydrate-related mixtures and a comparison of two association models.** Journal of Chemical and Engineering Data, Vol. 62, No. 9, 2017, pp. 2592-2605.

Liang, Xiaodong; Michelsen, Michael Locht / **General approach for solving the density gradient theory in the interfacial tension calculations.** Fluid Phase Equilibria, Vol. 451, 2017, pp. 79-90.

Liu, Ming; Ale, Marcel Tutor; Kołaczkowski, Bartłomiej; Fernando, Dinesh; Daniel, Geoffrey; Meyer, Anne S.; Thygesen, Anders / **Comparison of traditional field retting and Phlebia radiata Cel 26 retting of hemp fibres for fibre-reinforced composites.** A M B Express, Vol. 7, 58, 2017.

Liu, Xiaoyan; Feilberg, Karen Louise; Yan, Wei; Stenby, Erling Halfdan; Thormann, Esben / **Electrical double-layer and ion bridging forces between symmetric and asymmetric charged surfaces in the presence of mono- and divalent ions.** Langmuir, Vol. 33, No. 18, 2017, pp. 4426-4434.

Liu, Yanrong; Meyer, Anne S.; Nie, Yi; Zhang, Suojiang; Zhao, Yongsheng; Fosbøl, Philip Loldrup; Thomsen, Kaj / **Freezing point determination of water-ionic liquid mixtures.** Journal of Chemical and Engineering Data, Vol. 62, No. 8, 2017, pp. 2374-2383.

Liu, Ming; Baum, Andreas; Odermatt, Jürgen; Berger, Jens; Yu, Liyun; Zeuner, Birgitte; Thygesen, Anders; Holck, Jesper; Meyer, Anne S. / **Oxidation of lignin in hemp fibres by laccase: effects on mechanical properties of hemp fibres and unidirectional fibre/epoxy composites.** Composites Part A: Applied Science and Manufacturing, Vol. 95, 2017, pp. 377-387.

Liu, Ming; Thygesen, Anders; Summerscales, John; Meyer, Anne S. / **Targeted pre-treatment of hemp bast fibres for optimal performance in biocomposite materials: A review.** Industrial Crops and Products, Vol. 108, 2017, pp. 660-683.

Loureiro da Costa Lira Gargalo, Carina; Carvalho, Ana; Gernaey, Krist V.; Sin, Gürkan / **Optimal design and planning of glycerol-based biorefinery supply chains under uncertainty.** Industrial & Engineering Chemistry Research, Vol. 56, No. 41, 2017, pp. 11870-11893.

Loureiro da Costa Lira Gargalo, Carina; Carvalho, Ana; Gernaey, Krist; Sin, Gürkan / **Supply chain optimization of integrated glycerol biorefinery: glythink model development and application.** Industrial and Engineering Chemistry Research, Vol. 56, No. 23, 2017, pp. 6711-6727.

Lu, Zhimin; Jian, Jie; Jensen, Peter Arendt; Wu, Hao; Glarborg, Peter / **Impact of KCl impregnation on single particle combustion of wood and torrefied wood.** Fuel, Vol. 206, 2017, pp. 684-689.

Lu, Bona; Zhang, Jingyuan; Luo, Hao; Wang, Wei; Li, Hua; Ye, Mao; Liu, Zhongmin; Li, Jinghai / **Numerical simulation of scale-up effects of methanol-to-olefins fluidized bed reactors.** Chemical Engineering Science, Vol. 171, 2017, pp. 244-255.

Luo, Hao; Lu, Bona; Zhang, Jingyuan; Wu, Hao; Wang, Wei / **A grid-independent EMMS/bubbling drag model for bubbling and turbulent fluidization.** Chemical Engineering Journal, Vol. 326, 2017, pp. 47-57.

Lymperatou, Anna; Gavala, Hariklia N; Skiadas, Ioannis / **Optimization of aqueous ammonia soaking of manure fibers by response surface methodology for unlocking the methane potential of swine manure.** Bioresource Technology, Vol. 244, 2017, pp. 509-516.

Lythcke-Jørgensen, Christoffer Ernst; Clausen, Lasse Røngaard; Algren, Loui; Bavnhøj Hansen, Anders; Münster, Marie; Gadsbøll, Rasmus Østergaard; Haglind, Fredrik / **Optimization of a flexible multi-generation system based on wood chip gasification and methanol production.** Applied Energy, Vol. 192, 2017, pp. 337-359.

Mackay, Jessica E.; Cavagnaro, Timothy R.; Jakobsen, Iver; Macdonald, Lynne M.; Grønlund, Mette; Thomsen, Tobias Pape; Müller-Stöver, Dorette S. / **Evaluation of phosphorus in thermally converted sewage sludge: P pools and availability to wheat.** Plant and Soil, Vol. 418, No. 1-2, 2017, pp. 307-317.

Manns, Dirk Martin; Nielsen, Mette Møller; Bruhn, Annette; Saake, Bodo; Meyer, Anne S. / **Compositional variations of brown seaweeds Laminaria digitata and Saccharina latissima in Danish waters.** Journal of Applied Phycology, Vol. 29, No. 3, 2017, pp. 1493-1506.

Mansouri, Seyed Soheil; S.B.A. Udugama, Isuru; Cignitti, Stefano; Mitic, Aleksandar; Flores Alsina, Xavier; Gernaey, Krist / **Resource recovery from bio-based production processes: A future necessity?** Current Opinion in Chemical Engineering, Vol. 18, 2017, pp. 1-9.

Marpani, Fauziah Binti; Pinelo, Manuel; Meyer, Anne S. / **Enzymatic conversion of $CO_2$ to $CH_3OH$ via reverse dehydrogenase cascade biocatalysis: Quantitative comparison of efficiencies of immobilized enzyme systems.** Biochemical Engineering Journal, Vol. 127, 2017, pp. 217-228.

Marpani, Fauziah Binti; Sárossy, Zsuzsa ; Pinelo, Manuel; Meyer, Anne S. / **Kinetics based reaction optimization of enzyme catalysed reduction of formaldehyde to methanol with synchronous cofactor regeneration.** Biotechnology and Bioengineering, Vol. 114, No. 12, 2017, pp. 2762-2770.

Mears, Lisa; Stocks, Stuart M.; Albæk, Mads Orla; Sin, Gürkan; Gernaey, Krist V. / **Application of a mechanistic model as a tool for on-line monitoring of pilot scale filamentous fungal fermentation processes - the importance of evaporation effects : Mechanistic model for pilot scale monitoring.** Biotechnology and Bioengineering, Vol. 114, No. 3, 2017, pp. 589-599.

Mears, Lisa; Stocks, Stuart M.; Albaek, Mads O.; Cassells, Benny; Sin, Gürkan; Gernaey, Krist / **A novel model-based control strategy for aerobic filamentous fungal fed-batch fermentation processes.** Biotechnology and Bioengineering (Print), Vol. 114, No. 7, 2017, pp. 1459-1468.

Mears, Lisa; Stocks, Stuart M.; Sin, Gürkan; Gernaey, Krist / **A review of control strategies for manipulating the feed rate in fed-batch fermentation processes.** Journal of Biotechnology, Vol. 245, 2017, pp. 34-46.

Mears, Lisa; Stocks, Stuart M; Albæk, Mads Orla; Sin, Gürkan; Gernaey, Krist V. / **Mechanistic fermentation models for process design, monitoring, and control.** Trends in Biotechnology, Vol. 35, No. 10, 2017, pp. 914-924.

Miezah, Kodwo; Obiri-Danso, Kwasi; Kádár, Zsófia; Heiske, Stefan; Fei-Baffoe, Bernard; Mensah, Moses; Meyer, Anne S. / **Municipal solid waste management in a low income economy through biogas and bioethanol production.** Waste and Biomass Valorization, Vol. 8, No. 1, 2017, pp. 115-127.

Mitic, Aleksandar; Skov, Thomas; Gernaey, Krist V. / **Removal of benzaldehyde from a water/ethanol mixture by applying scavenging techniques.** Green Processing and Synthesis, Vol. 6, No. 3, 2017, pp. 353-361.

Mohd Sueb, Mohd Shafiq Bin; Luo, Jianquan; Meyer, Anne S.; Jørgensen, Henning; Pinelo, Manuel / **Impact of the fouling mechanism on enzymatic depolymerization of xylan in different configurations of membrane reactors.** Separation and Purification Technology, Vol. 178, 2017, pp. 154-162.

Mollerup, Ane Loft; Mikkelsen, Peter Steen; Thornberg, D.; Sin, Gürkan / **Controlling sewer systems – a critical review based on systems in three EU cities.** Urban Water Journal, Vol. 14, No. 4, 2017, pp. 435-442.

Montagud, Maria E. Mondejar; Cignitti, Stefano; Abildskov, Jens; Woodley, John; Haglind, Fredrik / **Prediction of properties of new halogenated olefins using two group contribution approaches.** Fluid Phase Equilibria, Vol. 433, 2017, pp. 79-96.

Morthensen, Sofie Thage; Sigurdardóttir, Sigyn Björk; Meyer, Anne S.; Jørgensen, Henning; Pinelo, Manuel / **Separation of xylose and glucose using an integrated membrane system for enzymatic cofactor regeneration and downstream purification.** Journal of Membrane Science, Vol. 523, 2017, pp. 327-335.

Morthensen, Sofie Thage; Meyer, Anne S.; Jørgensen, Henning; Pinelo, Manuel / **Significance of membrane bioreactor design on the biocatalytic performance of glucose oxidase and catalase: Free vs. immobilized enzyme systems.** Biochemical Engineering Journal, Vol. 117, 2017, pp. 41-47.

Møller, Victor Buhl; Dam-Johansen, Kim; Frankær, Sarah Maria Grundahl; Kiil, Søren / **Acid-resistant organic coatings for the chemical industry: A review.** Journal of Coatings Technology and Research, Vol. 14, No. 2, 2017, pp. 279-306.

Mu, Liang; von Solms, Nicolas / **Methane production and carbon capture by hydrate swapping.** Energy & Fuels, Vol. 31, No. 4, 2017, pp. 3338-3347.

Munk, Line; Andersen, Mogens Larsen; Meyer, Anne S. / **Direct rate assessment of laccase catalysed radical formation in lignin by electron paramagnetic resonance spectroscopy.** Enzyme and Microbial Technology, Vol. 106, 2017, pp. 88-96.

Munk, Line; Punt, A. M.; Kabel, M. A.; Meyer, Anne S. / **Laccase catalyzed grafting of-N-OH type mediators to lignin via radical-radical coupling.** RSC Advances, Vol. 7, No. 6, 2017, pp. 3358-3368.

Nakayama, Ryo-ichi; Imai, Masanao; Woodley, John / **Ultrasound-assisted production of biodiesel FAME from rapeseed oil in a novel two-compartment reactor.** Journal of Chemical Technology and Biotechnology, Vol. 92, No. 3, 2017, pp. 657-665.

Neergaard, Jesper S; Møller, Katrine Dragsbæk; Christiansen, Claus; Nielsen, Henning B.; Pedersen, Susanne Brix; Karsdal, Morten Asser; Henriksen, Kim / **Metabolic syndrome, insulin resistance and cognitive dysfunction: Does your metabolic profile affect your brain?** Diabetes, Vol. 66, No. 4, db161444, 2017.

Nielsen, Joachim Bachmann; Jensen, Anders; Madsen, Line Riis; Larsen, Flemming H.; Felby, Claus; Jensen, Anker Degn / **Noncatalytic direct liquefaction of biorefinery lignin by ethanol.** Energy and Fuels, Vol. 31, No. 7, 2017, pp. 7223-7233.

Nielsen, Rasmus Fjordbak; Huusom, Jakob Kjøbsted; Abildskov, Jens / **Driving force based design of cyclic distillation.** Industrial and Engineering Chemistry Research, Vol. 56, No. 38, 2017, pp. 10833-10844.

Nimmanterdwong, Prathana; Chalermsinsuwan, Benjapon; Østergård, Hanne; Piumsomboon, Pornpote / **Environmental performance assessment of Napier grass for bioenergy production.** Journal of Cleaner Production, Vol. 165, 2017, pp. 645-655.

Noguer, Albert Camós; Olsen, A.; Hvilsted, Søren; Kiil, Søren / **Field study of the long-term release of block copolymers from fouling-release coatings.** Progress in Organic Coatings, Vol. 112, 2017, pp. 101-108.

Noguer, Albert Camós; Olsen, S. M.; Hvilsted, Søren; Kiil, Søren / **Diffusion of surface-active amphiphiles in silicone-based fouling-release coatings.** Progress in Organic Coatings, Vol. 106, 2017, pp. 77-86.

Nyffenegger, Christian; Nordvang, Rune Thorbjørn; Jers, Carsten; Meyer, Anne S.; Mikkelsen, Jørn Dalgaard / **Design of Trypanosoma rangeli sialidase mutants with improved trans-sialidase activity.** PLOS ONE, Vol. 12, No. 2, e0171585, 2017.

Okoro, Sunday Chukwudi; Kiamehr, Saeed; Montgomery, Melanie; Jappe Frandsen, Flemming; Pantleon, Karen / **Effect of flue gas composition on deposit induced high temperature corrosion under laboratory conditions mimicking biomass firing. Part I: Exposures in oxidizing and chlorinating atmospheres.** Materials and Corrosion, Vol. 68, No. 15, 2017, pp. 499-514.

Okoro, Sunday Chukwudi; Kiamehr, Saeed; Montgomery, Melanie; Jappe Frandsen, Flemming; Pantleon, Karen / **Effect of flue gas composition on deposit induced high temperature corrosion under laboratory conditions mimicking biomass firing. Part II: Exposures in $SO_2$ containing atmospheres.** Materials and Corrosion, Vol. 68, No. 5, 2017, pp. 515-528.

Okoro, Sunday Chukwudi; Kvisgaard, M.; Montgomery, Melanie; Jappe Frandsen, Flemming; Pantleon, Karen / **Pre-oxidation and its effect on reducing high-temperature corrosion of superheater tubes during biomass firing.** Surface Engineering, Vol. 33, No. 6, 2017, pp. 428-432.

Okoro, Sunday Chukwudi; Montgomery, Melanie; Jappe Frandsen, Flemming; Pantleon, Karen / **Influence of preoxidation on high temperature corrosion of a Ni-based alloy under conditions relevant to biomass firing.** Surface and Coatings Technology, Vol. 319, 2017, pp. 76-87.

Okoro, Sunday Chukwudi; Nießen, Frank; Villa, Matteo; Apel, Daniel; Montgomery, Melanie; Jappe Frandsen, Flemming; Pantleon, Karen / **Complementary methods for the characterization of corrosion products on a plant-exposed superheater tube.** Metallography, Microstructure, and Analysis, Vol. 6, No. 1, 2017, pp. 22-35.

Olsen, Brian Kjærgaard; Castellino, Francesco; Jensen, Anker Degn / **Modeling deactivation of catalysts for selective catalytic reduction of NOx by KCl aerosols.** Industrial and Engineering Chemistry Research, Vol. 56, No. 45, 2017, pp. 13020-13033.

Pang, Kar Mun; Karvounis, Nikolas; Walther, Jens Honore; Schramm, Jesper; Glarborg, Peter; Mayer, Stefan / **Modelling of temporal and spatial evolution of sulphur oxides and sulphuric acid under large, two-stroke marine engine-like conditions using integrated CFD-chemical kinetics.** Applied Energy, Vol. 193, 2017, pp. 60-73.

Papadakis, Emmanouil; Anantpinijwatna, Amata; Woodley, John; Gani, Rafiqul / **A reaction database for small molecule pharmaceutical processes integrated with process information.** Processes, Vol. 5, No. 5, 58, 2017.

Papadakis, Emmanouil; Pedersen, Sven; Kumar Tula, Anjan; Fedorova, Marina; Woodley, John; Gani, Rafiqul / **Model-based design and analysis of glucose isomerization process operation.** Chemical Engineering, Vol. 98, 2017, pp. 128-142.

Parés Viader, Raimon; Jensen, Pernille Erland; Ottosen, Lisbeth M.; Ahrenfeldt, Jesper; Hauggaard-Nielsen, Henrik / **Sequential electrodialytic recovery of phosphorus from low-temperature gasification ashes of chemically precipitated sewage sludge.** Waste Management, Vol. 60, 2017, pp. 211-218.

Parés Viader, Raimon; Jensen, Pernille Erland; Ottosen, Lisbeth M.; Thomsen, Tobias Pape; Ahrenfeldt, Jesper; Hauggaard-Nielsen, Henrik / **Comparison of phosphorus recovery from incineration and gasification sewage sludge ash.** Water Science and Technology, Vol. 75, No. 5, 2017, pp. 1251-1260.

Paterson, Duncan; Michelsen, Michael Locht; Yan, Wei; Stenby, Erling Halfdan / **Extension of modified RAND to multiphase flash specifications based on state functions other than (T,P).** Fluid Phase Equilibria, Vol. 458, 2017, pp. 288-299.

Pedersen, Asbjørn Toftgaard; Teresa de Melo Machado Simoes Carvalho, Ana; Sutherland, Euan; Rehn, Gustav; Ashe, Robert; Woodley, John / **Characterization of a continuous agitated cell reactor for oxygen dependent biocatalysis.** Biotechnology and Bioengineering, Vol. 114, No. 6, 2017, pp. 1222-1230.

Pedersen, Morten Nedergaard; Nielsen, Mads; Clausen, Sønnik; Jensen, Peter Arendt; Jensen, Lars Skaarup; Dam-Johansen, Kim / **Imaging of flames in cement kilns to study the influence of different fuel types.** Energy and Fuels, Vol. 31, No. 10, 2017, pp. 11424-11438.

Pereira Rosinha Grundtvig, Ines; Daugaard, Anders Egede; Woodley, John; Gernaey, Krist; Krühne, Ulrich / **Shape optimization as a tool to design biocatalytic microreactors.** Chemical Engineering Journal, Vol. 322, 2017, pp. 215-223.

Perrin, Aurelie; Wohlfahrt, Julie; Morandi, Fabiana; Østergård, Hanne; Flatberg, Truls; De La Rua, Cristina; Bjørkvoll, Thor; Gabrielle, Benoit / **Integrated design and sustainable assessment of innovative biomass supply chains: A case-study on miscanthus in France.** Applied Energy, Vol. 204, 2017, pp. 66-77.

Petersen, Leander Adrian Haaning; Villadsen, John; Jørgensen, Sten Bay; Gernaey, Krist / **Mixing and mass transfer in a pilot scale U-loop bioreactor.** Biotechnology and Bioengineering, Vol. 114, No. 2, 2017, pp. 344-354.

Pierce, Brian; Wittrup Agger, Jane; Zhang, Zhenghong; Wichmann, Jesper; Meyer, Anne S. / **A comparative study on the activity of fungal lytic polysaccharide monooxygenases for the depolymerization of cellulose in soybean spent flakes.** Carbohydrate Research, Vol. 449, 2017, pp. 85-94.

Pierce, Brian; Wittrup Agger, Jane; Wichmann, Jesper; Meyer, Anne S. / **Oxidative cleavage and hydrolytic boosting of cellulose in soybean spent flakes by Trichoderma reesei Cel61A lytic polysaccharide monooxygenase.** Enzyme and Microbial Technology, Vol. 98, 2017, pp. 58-66.

Pinto Coelho Muniz Vinhal, Andre; Yan, Wei; Kontogeorgis, Georgios / **Evaluation of equations of state for simultaneous representation of phase equilibrium and critical phenomena.** Fluid Phase Equilibria, Vol. 437, 2017, pp. 140-154.

Pitt, John I.; Lange, Lene; Lacey, Alastair E.; Vuong, Daniel; Midgley, David J.; Greenfield, Paul; Bradbury, Mark I.; Lacey, Ernest; Busk, Peter Kamp; Pilgaard, Bo; Chooi, Yit Heng; Piggott, Andrew M. / **Aspergillus hancockii sp. Nov., a biosynthetically talented fungus endemic to southeastern Australian soils.** PLoS ONE, Vol. 12, No. 4, e0170254, 2017.

Prunescu, Remus Mihail; Blanke, Mogens; Jakobsen, Jon Geest; Sin, Gürkan / **Model-based plant-wide optimization of large-scale lignocellulosic bioethanol plants.** Biochemical Engineering Journal, Vol. 124, 2017, pp. 13-25.

Puig Arnavat, Maria; Ahrenfeldt, Jesper; Henriksen, Ulrik Birk / **Validation of a multiparameter model to investigate torrefied biomass pelletization behavior.** Energy & Fuels, Vol. 31, No. 2, 2017, pp. 1644-1649.

Ramin, Pedram; Valverde Pérez, Borja; Polesel, Fabio; Locatelli, Luca; Plósz, Benedek G. / **A systematic model identification method for chemical transformation pathways - the case of heroin biomarkers in wastewater.** Scientific Reports, Vol. 7, No. 1, 9390, 2017.

Ramin, Pedram; Brock, Andreas Libonati; Causanilles Llanes, Ana; Valverde Pérez, Borja; Emke, Erik; de Voogt, Pim; Polesel, Fabio; Plósz, Benedek G. / **Transformation and sorption of illicit drug biomarkers in sewer biofilms.** Environmental Science and Technology, Vol. 51, No. 18, 2017, pp. 10572-10584.

Rasmussen, Dominik Bjørn; Christensen, Jakob Munkholt; Temel, B.; Studt, F.; Moses, P.G.; Rossmeisl, Jan; Riisager, Anders; Jensen, Anker Degn / **Reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite: A combined DFT/experimental study.** Catalysis Science & Technology, Vol. 7, No. 5, 2017, pp. 1141-1152.

Rasmussen, H.; Tanner, David Ackland; Sørensen, H. R.; Meyer, Anne S. / **New degradation compounds from lignocellulosic biomass pretreatment: Routes for formation of potent oligophenolic enzyme inhibitors.** Green Chemistry, Vol. 19, 2017, pp. 464-473.

Rasmussen, H.; Sørensen, Henrik Rokkjær; Tanner, David Ackland; Meyer, Anne S. / **New pentose dimers with bicyclic moieties from pretreated biomass.** R S C Advances, Vol. 7, No. 9, 2017, pp. 5206-5213.

Rasmussen, Henrik Koblitz; Huang, Qian / **Constant interchain pressure effect in extensional flows of oligomer diluted polystyrene and poly(methyl methacrylate) melts.** Rheologica Acta, Vol. 56, No. 1, 2017, pp. 27-34.

Regueira, Teresa; Lugo, Luis; Comuñas, María J. P.; Fernández, Josefa / **High pressure rheological behavior of 1-ethyl-3-methylimidazolium n-hexylsulfate and trihexyl(tetradecyl)phosphonium tris(pentafluoroethyl)trifluorophosphate.** Journal of Chemical and Engineering Data, Vol. 62, No. 9, 2017, pp. 2927-2936.

Regueira Muñiz, Teresa; Liu, Yiqun; Wibowo, Ahmad A.; Ashrafi, Mehrshad; Varzandeh, Farhad; Pantelide, Georgia; Stenby, Erling Halfdan; Yan, Wei / **High pressure phase equilibrium of ternary and multicomponent alkane mixtures in the temperature range from (283-473) K.** Fluid Phase Equilibria, Vol. 449, 2017, pp. 186-196.

Reinhardt, Juliane; Hoppe, Robert; Hofmann, Georg; Damsgaard, Christian Danvad; Patommel, Jens; Baumbach, Christoph; Baier, Sina; Rochet, Amélie; Grunwaldt, Jan-Dierk; Falkenberg, Gerald; Schroer, Christian G. / **Beamstop-based low-background ptychography to image weakly scattering objects.** Ultramicroscopy, Vol. 173, 2017, pp. 52-57.

Rhein-Knudsen, Nanna; Ale, Marcel Tutor; Ajalloueian, Fatemeh; Meyer, Anne S. / **Characterization of alginates from Ghanaian brown seaweeds: Sargassum spp. and Padina spp.** Food Hydrocolloids, Vol. 71, 2017, pp. 236-244.

Rhein-Knudsen, Nanna; Ale, Marcel Tutor; Ajalloueian, Fatemeh; Yu, Liyun; Meyer, Anne S. / **Rheological properties of agar and carrageenan from Ghanaian red seaweeds.** Food Hydrocolloids, Vol. 63, 2017, pp. 50-58.

Ringborg, Rolf Hoffmeyer; Pedersen, Asbjørn Toftgaard; Woodley, John / **Automated determination of oxygen-dependent enzyme kinetics in a tube-in-tube flow reactor.** Chemcatchem, Vol. 9, 2017, pp. 3285-3288.

Rousis, Nikolaos I.; Gracia-Lor, Emma; Zuccato, Ettore; Bade, Richard; Baz-Lomba, Jose Antonio; Castrignanò, Erika; Causanilles, Ana; Covaci, Adrian; de Voogt, Pim; Hernández, Félix; Kasprzyk-Hordern, Barbara; Kinyua, Juliet; McCall, Ann-Kathrin; Plósz, Benedek G.; Ramin, Pedram; Ryu, Yeonsuk; Thomas, Kevin V.; van Nuijs, Alexander; Yang, Zhugen; Castiglioni, Sara / **Wastewater-based epidemiology to assess pan-European pesticide exposure.** Water Research, Vol. 121, 2017, pp. 270-279.

Ruszczynski, Lukasz; Zubov, Alexandr; O'Connell, John P.; Abildskov, Jens / **Reliable correlation for liquid-liquid equilibria outside the critical region.** Journal of Chemical and Engineering Data, Vol. 62, No. 9, 2017, pp. 2842-2854.

Ruszczyński, Łukasz; Zubov, Alexandr; O'Connell, John P.; Abildskov, Jens / **Reply to "Comment on 'Reliable correlation for liquid-liquid equilibria outside the critical region'".** Journal of Chemical and Engineering Data, Vol. 62, No. 11, 2017, pp. 4043-4044.

Rydahl, Maja Gro; Kračun, Stjepan K.; Fangel, Jonatan U.; Michel, Gurvan; Guillouzo, Alexia; Génicot, Sabine; Mravec, Jozef; Harholt, Jesper; Wilkens, Casper; Motawia, Mohammed Saddik; Svensson, Birte; Tranquet, Olivier; Ralet, Marie-Christine; Jørgensen, Bodil; Domozych, David S.; Willats, William G. T. / **Development of novel monoclonal antibodies against starch and ulvan - implications for antibody production against polysaccharides with limited immunogenicity.** Scientific Reports, Vol. 7, No. 1, 9326, 2017.

Saagi, Ramesh; Flores Alsina, Xavier; Kroll, J. S.; Gernaey, Krist; Jeppsson, U. / **A model library for simulation and benchmarking of integrated urban wastewater systems.** Environmental Modelling & Software, Vol. 93, 2017, pp. 282-295.

Sadegh, Negar; Stenby, Erling Halfdan; Thomsen, Kaj / **Thermodynamic modelling of acid gas removal from natural gas using the Extended UNIQUAC model.** Fluid Phase Equilibria, Vol. 442, 2017, pp. 38-43.

Sawers, Ruairidh J. H.; Svane, Simon; Quan, Clement; Grønlund, Mette; Wozniak, Barbara; Gebreselassie, Mesfin-Nigussie; González-Muñoz, Eliécer; Chávez Montes, Ricardo A; Baxter, Ivan; Goudet, Jerome; Jakobsen, Iver; Paszkowski, Uta / **Phosphorus acquisition efficiency in arbuscular mycorrhizal maize is correlated with the abundance of root-external hyphae and the accumulation of transcripts encoding PHT1 phosphate transporters.** New Phytologist, Vol. 214, No. 2, 2017, pp. 632-643.

S.B.A. Udugama, Isuru; Mansouri, Seyed Soheil; Mitic, Aleksandar; Flores Alsina, Xavier; Gernaey, Krist V. / **Perspectives on resource recovery from bio-based production processes: From concept to implementation.** Processes, Vol. 5, 48, 2017.

Scherz, Leon F.; Costanzo, Salvatore; Huang, Qian; Schlutter, A. Dieter; Vlassopoulos, Dimitris / **Dendronized polymers with ureidopyrimidinone groups: An efficient strategy to tailor intermolecular interactions, rheology, and fracture.** Macromolecules, Vol. 50, No. 13, 2017, pp. 5176-5187.

Schlaikjer, Anders; Thomsen, Kaj; Kontogeorgis, Georgios / **Simultaneous description of activity coefficients and solubility with eCPA.** Industrial and Engineering Chemistry Research, Vol. 56, No. 4, 2017, pp. 1074-1089.

Shabbir, Aamir; Huang, Qian; P. Baeza, Guilhem ; Vlassopoulos, Dimitris; Chen, Quan; H. Colby, Ralph ; J. Alvarez, Nicolas; Hassager, Ole / **Non-linear shear and uniaxial extensional rheology of polyether-ester-sulfonate copolymer ionomer melts.** Journal of Rheology, Vol. 61, 2017, pp. 1279-1289.

Shahid, T.; Huang, Qian; Oosterlinck, F.; Clasen, C.; van Ruymbeke, E. / **Dynamic dilution exponent in monodisperse entangled polymer solutions.** Soft Matter, Vol. 13, 2017, pp. 269-282.

Shcherbakov, Nataliya ; Rodriguez-Donis, Ivonne; Abildskov, Jens; Gerbaud, Vincent / **A novel method for detecting and computing univolatility curves in ternary mixtures.** Chemical Engineering Science, Vol. 173, 2017, pp. 21-36.

Siedler, Solvej; Khatri, Narendar K.; Zsohar, Andrea; Kjærbølling, Inge; Vogt, Michael; Hammar, Petter; Nielsen, Christian Førgaard; Marienhagen, Jan; Sommer, Morten Otto Alexander; Joensson, Haakan N. / **Development of a bacterial biosensor for rapid screening of yeast p-coumaric acid production.** A C S Synthetic Biology, Vol. 6, No. 10, 2017, pp. 1860-1869.

Siirola, Jeffrey; Gani, Rafiqul / **Preface.** Computers & Chemical Engineering, Vol. 105, 2017, pp. 1.

Solon, Kimberly ; Flores Alsina, Xavier; Kazadi Mbamba, C; Ikumi, David; Volcke, E.I.P.; Vaneeckhaute, C; Ekama, G.; Vanrolleghem, P A; Batstone, Damien J.; Gernaey, Krist; Jeppsson, U / **Plant-wide modelling of phosphorus transformations in wastewater treatment systems: Impacts of control and operational strategies.** Water Research, Vol. 113, 2017, pp. 97-110.

Sonnenschein, Eva Christina; Phippen, Christopher Broughton William; Nielsen, Kristian Fog; Mateiu, Ramona Valentina; Melchiorsen, Jette; Gram, Lone; Overmann, Jörg; Freese, Heike M / **Phaeobacter piscinae sp. nov., a species of the Roseobacter group and potential aquaculture probiont.** International Journal of Systematic and Evolutionary Microbiology, Vol. 67, No. 10, 2017.

Sueb, Mohd Shafiq Mohd; Zdarta, Jakub; Jesionowski, Teofil; Jonsson, Gunnar; Meyer, Anne S.; Jørgensen, Henning; Pinelo, Manuel / **High-performance removal of acids and furans from wheat straw pretreatment liquid by diananofiltration.** Separation Science and Technology (Philadelphia), Vol. 52, No. 11, 2017, pp. 1901-1912.

Thomsen, Tobias Pape; Sárossy, Zsuzsa ; Ahrenfeldt, Jesper; Henriksen, Ulrik Birk; Jappe Frandsen, Flemming; Müller-Stöver, Dorette Sophie / **Changes imposed by pyrolysis, thermal gasification and incineration on composition and phosphorus fertilizer quality of municipal sewage sludge.** Journal of Environmental Management, Vol. 198, 2017, pp. 308-318.

Thomsen, Tobias Pape; Sárossy, Zsuzsa; Gøbel, Benny; Stoholm, Peder; Ahrenfeldt, Jesper; Jappe Frandsen, Flemming; Henriksen, Ulrik Birk / **Low temperature circulating fluidized bed gasification and co-gasification of municipal sewage sludge. Part 1: Process performance and gas product characterization.** Waste Management, Vol. 66, 2017, pp. 123-133.

Thomsen, Tobias Pape; Hauggaard-Nielsen, Henrik; Gøbel, Benny; Stoholm, Peder; Ahrenfeldt, Jesper; Henriksen, Ulrik Birk; Müller-Stöver, Dorette Sophie / **Low temperature circulating fluidized bed gasification and co-gasification of municipal sewage sludge. Part 2: Evaluation of ash materials as phosphorus fertilizer.** Waste Management, Vol. 66, 2017, pp. 145-154.

Trifol Guzman, Jon; Sillard, Cecile; Plackett, D.; Szabo, Peter; Bras, Julien; Daugaard, Anders Egede / **Chemically extracted nanocellulose from sisal fibres by a simple and industrially relevant process.** Cellulose, Vol. 24, No. 1, 2017, pp. 107-118.

Tristan Djajadi, Demi; Hansen, Aleksander R.; Jensen, Anders; Thygesen, Lisbeth G.; Pinelo, Manuel; Meyer, Anne S.; Jørgensen, Henning / **Surface properties correlate to the digestibility of hydrothermally pretreated lignocellulosic Poaceae biomass feedstocks.** Biotechnology for Biofuels, Vol. 10, 49, 2017.

Trubetskaya, Anna; Surup, Gerrit; Shapiro, Alexander; B. Bates, Richard / **Modeling the influence of potassium content and heating rate on biomass pyrolysis.** Applied Energy, Vol. 194, 2017, pp. 199-211.

Trubetskaya, Anna; Surup, Gerrit; Shapiro, Alexander; B. Bates, Richard / **Publisher's Note to Modeling the influence of potassium content and heating rate on biomass pyrolysis [Appl. Energy J. 194 (2017) 199-211].** Applied Energy, Vol. 202, 2017, pp. 785.

Tsanas, Christos; Stenby, Erling Halfdan; Yan, Wei / **Calculation of multiphase chemical equilibrium by the modified RAND method.** Industrial and Engineering Chemistry Research, Vol. 56, No. 41, 2017, pp. 11983-11995.

Tsanas, Christos; Stenby, Erling Halfdan; Yan, Wei / **Calculation of simultaneous chemical and phase equilibrium by the method of Lagrange multipliers.** Chemical Engineering Science, Vol. 174, 2017, pp. 112-126.

Tsivintzelis, Ioannis; Kontogeorgis, Georgios; Panayiotou, Costas / **Dimerization of carboxylic acids: An equation of state approach.** Journal of Physical Chemistry Part B: Condensed Matter, Materials, Surfaces, Interfaces & Biophysical, Vol. 121, No. 9, 2017, pp. 2153-2163.

Van Bockstal, Pieter Jan; Mortier, Séverine Thérèse F.C.; Corver, Jos; Nopens, Ingmar; Gernaey, Krist V.; De Beer, Thomas / **Quantitative risk assessment via uncertainty analysis in combination with error propagation for the determination of the dynamic design space of the primary drying step during freeze-drying.** European Journal of Pharmaceutics and Biopharmaceutics, Vol. 121, 2017, pp. 32-41.

Van Daele, Timothy; Gernaey, Krist V.; Ringborg, Rolf Hoffmeyer; Börner, Tim; Heintz, Søren; Van Hauwermeiren, Daan; Grey, Carl; Krühne, Ulrich; Adlercreutz, Patrick; Nopens, Ingmar / **Application of iterative robust model-based optimal experimental design for the calibration of biocatalytic models.** Biotechnology Progress, Vol. 33, No. 5, 2017, pp. 1278-1293.

Varrone, Cristiano; Floriotis, Georgis; Heggeset, Tonje M. B.; Le, Simone B.; Markussen, Sidsel; Skiadas, Ioannis V; Gavala, Hariklia N. / **Continuous fermentation and kinetic experiments for the conversion of crude glycerol derived from second-generation biodiesel into 1,3 propanediol and butyric acid.** Biochemical Engineering Journal, Vol. 128, 2017, pp. 149-161.

Varrone, Cristiano; Heggeset, T. M. B.; Le, S. B. ; Haugen, T.; Markussen, S.; Skiadas, Ioannis V.; Gavala, Hariklia N. / **Corrigendum to "Comparison of different strategies for selection/adaptation of mixed microbial cultures able to ferment crude glycerol derived from second-generation biodiesel".** Journal of Biomedicine and Biotechnology, Vol. 2017, 2017, pp. 7602495.

Varzandeh, Farhad; Stenby, Erling Halfdan; Yan, Wei / **Comparison of GERG-2008 and simpler EoS models in calculation of phase equilibrium and physical properties of natural gas related systems.** Fluid Phase Equilibria, Vol. 434, 2017, pp. 21-43.

Varzandeh, Farhad; Stenby, Erling Halfdan; Yan, Wei / **General approach to characterizing reservoir fluids for EoS models using a large PVT database.** Fluid Phase Equilibria, Vol. 433, 2017, pp. 97-111.

Voges, Matthias; Abu, Rohana; Deslauriers, Maria Gundersen; Held, Christoph; Woodley, John; Sadowski, Gabriele / **Reaction equilibrium of the ω-transamination of (S)-phenylethylamine : Experiments and ePC-SAFT Modeling.** Organic Process Research and Development, Vol. 21, No. 7, 2017, pp. 976-986.

von Solms, Nicolas; Yan, Wei; Andersen, Simon / **17th International Conference on Petroleum Phase Behavior and Fouling.** Energy and Fuels, Vol. 31, No. 4, 2017, pp. 3329.

Wang, Bing-Yin; Liu, Yue-Xi; Weng, Jun-Jie; Glarborg, Peter; Tian, Zhen-Yu / **New insights in the low-temperature oxidation of acetylene.** Combustion Institute. Proceedings, Vol. 36, No. 1, 2017, pp. 355-363.

Wang, Yang; Wu, Hao; Sárossy, Zsuzsa ; Dong, Changqing; Glarborg, Peter / **Release and transformation of chlorine and potassium during pyrolysis of KCl doped biomass.** Fuel, Vol. 197, 2017, pp. 422-432.

Wang, Yuxin; Xiao, Feng-Shou; Seshan, Kulathu K.; Jensen, Anker Degn; Li, Yongdan / **Catalytic science and technology in sustainable energy II.** Catalysis Today, Vol. 298, 2017, pp. 1.

Wang, Ze; Zeng, Ying; Lin, Weigang; Song, Wenli / **In-situ hydrodeoxygenation of phenol by supported Ni catalyst-explanation for catalyst performance.** International Journal of Hydrogen Energy, Vol. 42, No. 33, 2017, pp. 21040-21047.

Wilkens, Casper; Andersen, Susan; Dumon, Claire; Berrin, Jean-Guy; Svensson, Birte / **GH62 arabinofuranosidases: Structure, function and applications.** Biotechnology Advances, Vol. 35, 2017, pp. 792-804.

Wilkens, Casper; Busk, Peter Kamp; Pilgaard, Bo; Zhang, Wen-Jing; Nielsen, Kåre L; Nielsen, Per Halkjær; Lange, Lene / **Diversity of microbial carbohydrate-active enzymes in Danish anaerobic digesters fed with wastewater treatment sludge.** Biotechnology for Biofuels, Vol. 10, 158, 2017.

Wingstrand, Sara Lindeblad; van Drongelen, Martin; Mortensen, Kell; S. Graham, Richard; Huang, Qian; Hassager, Ole / **Influence of extensional stress overshoot on crystallization of LDPE.** Macromolecules, Vol. 50, No. 3, 2017, pp. 1134-1140.

Wingstrand, Sara Lindeblad; Shen, Bo; Kornfield, Julie A.; Mortensen, Kell; Parisi, Daniele; Vlassopoulos, Dimitris; Hassager, Ole / **Rheological link between polymer melts with a high molecular weight tail and enhanced formation of shish-kebabs.** A C S Macro Letters, Vol. 6, 2017, p. 1268-1273.

Wittrup Agger, Jane; Busk, Peter Kamp; Pilgaard, Bo; Meyer, Anne S.; Lange, Lene / **A new functional classification of glucuronoyl esterases by peptide pattern recognition.** Frontiers in Microbiology, Vol. 8, 309, 2017.

Woodley, John / **Bioprocess intensification for the effective production of chemical products.** Computers & Chemical Engineering, Vol. 105, 2017, pp. 297-307.

Woodley, John M. / **Integrating protein engineering with process design for biocatalysis.** Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, Vol. 376, No. 2110, 20170062, 2017.

Xie, L.; Huang, T. L.; Wang, Y. H.; Zhang, L.; Wu, G. L.; Tsuji, N.; Huang, X. / **Structural refinement and property optimization in an Fe-23Cr-8.5Ni duplex stainless steel.** I O P Conference Series: Materials Science and Engineering, Vol. 219, 2017.

Xiros, Charilaos; Janssen, Matty; Bystrom, Roberth; Borresen, Borre T.; Cannella, David; Jørgensen, Henning; Koppram, Rakesh; Larsson, Christer; Olsson, Lisbeth; Tillman, Anne-Marie; Wannstrom, Sune / **Toward a sustainable biorefinery using high-gravity technology.** Biofuels, Bioproducts and Biorefining, Vol. 11, No. 1, 2017, pp. 15-27.

Yu, Liyun; Skov, Anne Ladegaard / **ZnO as a cheap and effective filler for high breakdown strength elastomers.** R S C Advances, Vol. 7, 45784, 2017.

Zakaria, Shamsul Bin; Madsen, Frederikke Bahrt; Skov, Anne Ladegaard / **Post curing as an effective means of ensuring the long-term reliability of PDMS thin films for dielectric elastomer applications.** Polymer-Plastics Technology and Engineering, Vol. 56, No. 1, 2017, pp. 83-95.

Zeuner, Birgitte; González-Delgado, Isabel; Holck, Jesper; Morales, Gabriel; López-Muñoz, María-José; Segura, Yolanda; Meyer, Anne S.; Mikkelsen, Jørn Dalgaard / **Characterization and immobilization of engineered sialidases from *Trypanosoma rangeli* for transsialylation.** Aims Molecular Science, Vol. 4, No. 2, 2017, pp. 140-163.

Zhao, Yongsheng; Gani, Rafiqul; Afzal, Raja Muhammad; Zhang, Xiangping; Zhang, Suojiang / **Ionic liquids for absorption and separation of gases: An extensive database and a systematic screening method.** A I Ch E Journal, Vol. 63, No. 4, 2017, pp. 1353-1367.

Zhou, Aijuan; Zhang, Jiaguang; Varrone, Cristiano; Wen, Kaili; Wang, Guoying; Liu, Wenzong; Wang, Aijie; Yue, Xiuping / **Process assessment associated to microbial community response provides insight on possible mechanism of waste activated sludge digestion under typical chemical pre-treatments.** Energy, Vol. 137, 2017, pp. 457-467.

Åberg, Andreas; Widd, Anders; Abildskov, Jens; Huusom, Jakob Kjøbsted / **Parameter estimation and analysis of an automotive heavy-duty SCR catalyst model.** Chemical Engineering Science, Vol. 161, 2017, pp. 167-177.

## Contributions to books

Cockburn, Darrell; Wilkens, Casper; Svensson, Birte / **Affinity Electrophoresis for Analysis of Catalytic Module-Carbohydrate Interactions.** Protein-Carbohydrate Interactions: Methods and Protocols. ed. / D. Wade Abbott; Alicia Lammerts van Bueren. Springer, Vol. 1588, 2017. pp. 119-127.

J. S. M. Silva, Carla; Prunescu, Remus Mihail; Gernaey, Krist; Sin, Gürkan; Diaz-Chavez, Rocio A. / **Biorefinery Sustainability Analysis.** Biorefineries - Targeting Energy, High Value Products. ed. / Miriam Rabaçal; Ana F. Ferreira; Carla A. M. Silva; Mário Costa. Springer, Vol. 57, 2017. pp. 161-200.

Gani, Rafiqul; Zhang, L.; Kalakul, Sawitree; Cignitti, Stefano / **Chapter 6 - Computer-Aided Molecular Design and Property Prediction.** Computer Aided Chemical Engineering: Tools For Chemical Product Design — From Consumer Products to Biomedicine. ed. / Mariano Martín; Mario R. Eden; Nishanth G. Chemmangattuvalappil. Elsevier Science, Vol. 39, 2017. pp. 153-196.

Kalakul, Sawitree; Cignitti, Stefano; Zhang, L.; Gani, Rafiqul / **Chapter 3 - VPPD-Lab: The Chemical Product Simulator.** Computer Aided Chemical Engineering: Tools For Chemical Product Design — From Consumer Products to Biomedicine. ed. / Mariano Martín; Mario R. Eden; Nishanth G. Chemmangattuvalappil. Elsevier Science, Vol. 39, 2017. pp. 61-94.

Lange, L.; Parmar, V.; Meyer, A. / **Biocatalysis.** Encyclopedia of Sustainable Technologies. ed. / M. A. Abraham. Oxford: Elsevier Science, Vol. 1, 2017. pp. 663-673.

Westereng, Bjørge; Arntzen, Magnus Ø.; Wittrup Agger, Jane; Vaaje-Kolstad, Gustav; Eijsink, Vincent G. H. / **Analyzing Activities of Lytic Polysaccharide Monooxygenases by Liquid Chromatography and Mass Spectrometry.** Protein-Carbohydrate Interactions: Methods and Protocols. ed. / D. Wade Abbott; Alicia Lammerts van Bueren. Springer, Vol. 1588, 2017. pp. 71-92.

## Books & Monographs

Skov, Anne Ladegaard / **Silicone-based Dielectric Elastomers.** Dr. Tech thesis. Kgs. Lyngby: Technical University of Denmark (DTU), 2017. 278 p.

## PhD theses defences

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## USEFUL INFORMATION

**POLYMER MEMBRANE**
Two kinds of monomer were polymerized with different ratio. The flexibility can be controlled by changing the ratio. The membrane can be used to separate $CO_2$ from $N_2$.

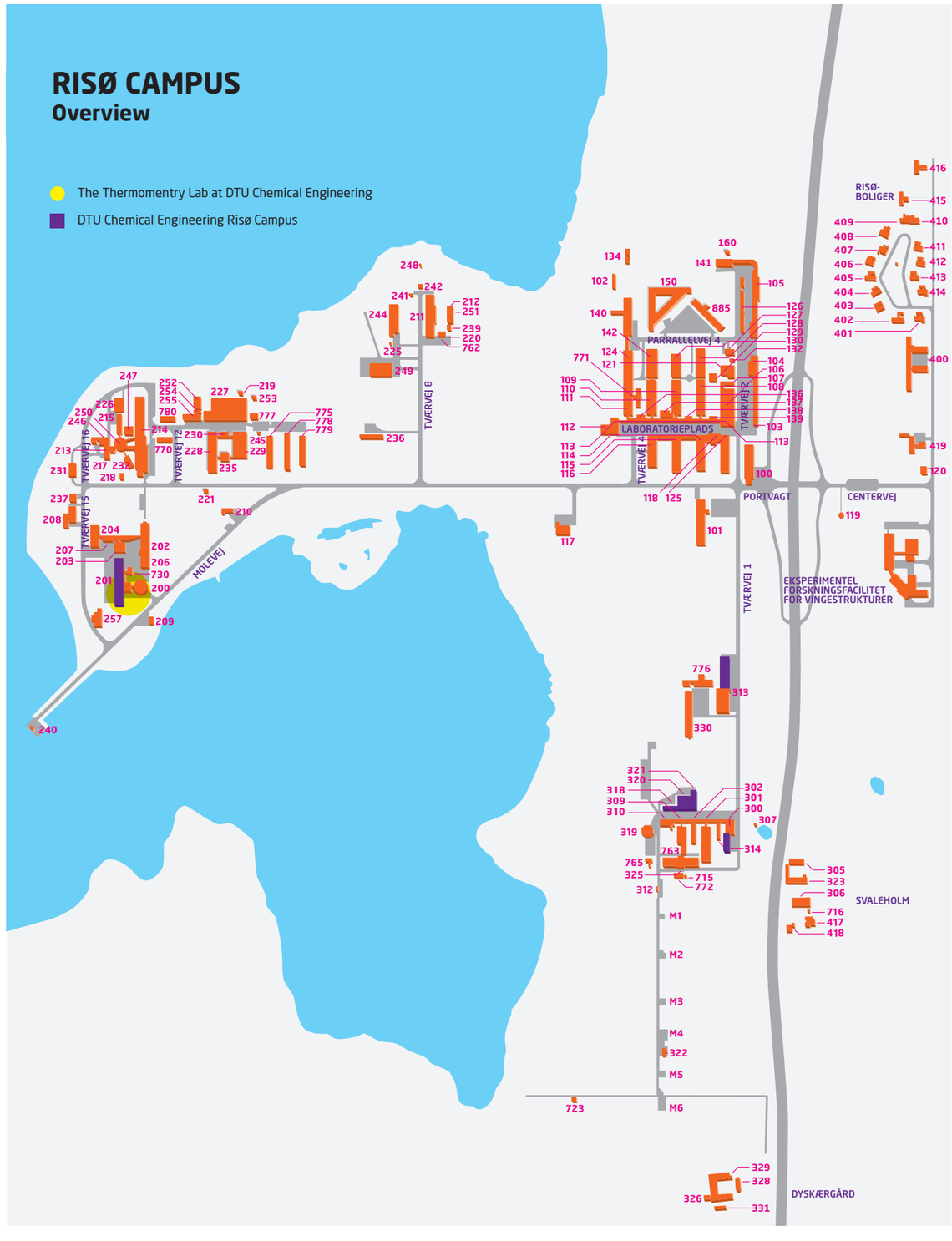
Photo: Thorkild Christensen

# LYNGBY CAMPUS
## Overview

- Department of Chemical and Biochemical Engineering
- Departments
- Oticon Hall
- Administration
- Campus Service
- Halls of Residence and guest houses
- Scion DTU
- Instructional buildings
- Bus stops
- Canteens
- DTU Library
- DTU Meeting Centre


# RISØ CAMPUS
## Overview

- The Thermomentry Lab at DTU Chemical Engineering
- DTU Chemical Engineering Risø Campus



Enzyme discovery is a key discipline at BioEng. Facilitated by computational tools, novel enzymes are discovered, characterized, and engineered with the aim to improve biomass valorisation.

Photo: Thorkild Christensen

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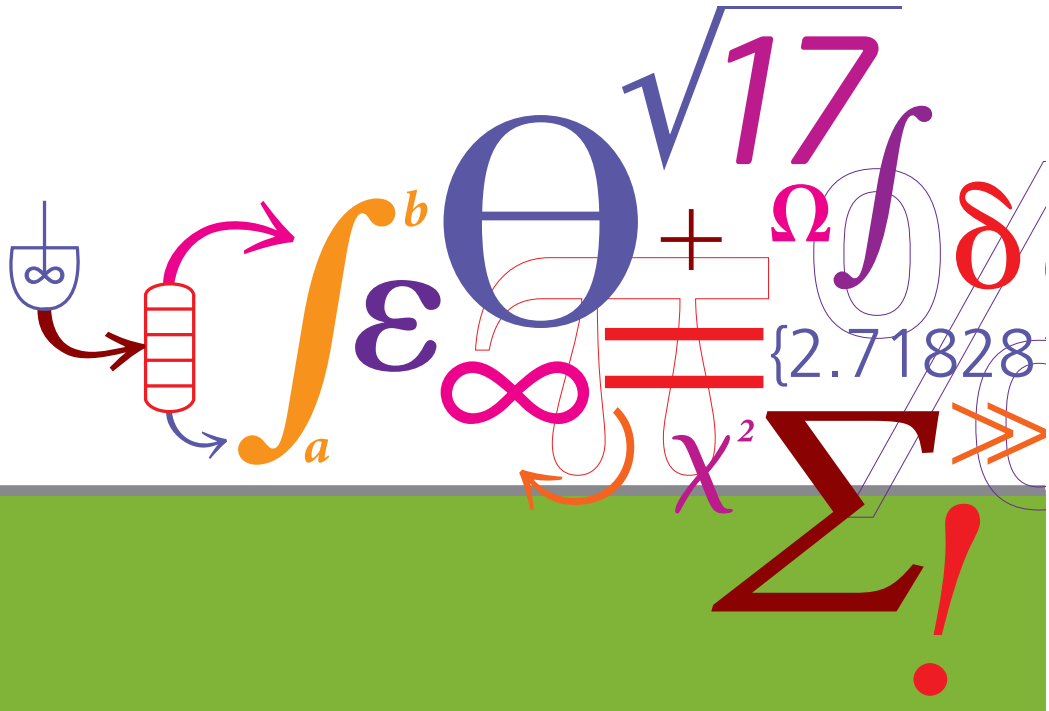


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