

# Annual Report 2016



# Key numbers of 2016

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 of 2016 to show how they support our strategic objectives.

STRATEGIC AREA	VISION	RESULTS IN 2016	
RESEARCH	Supports the development of sustainable solutions in the fields of chemistry, biotechnology, food, pharma, and energy through research and scientific advice.	<b>239</b> SCIENTIFIC ARTICLES IN WOS-INDEXED JOURNALS <b>3</b> BOOKS & MONOGRAPHS <b>12</b> CONTRIBUTIONS TO BOOKS <b>35</b> PHD THESES	
INNOVATION	An attractive partner for university departments and research-based industry.	<b>16</b> ACCEPTED PATENT IDEAS & SPIN-OUTS <b>8</b> INDUSTRIAL PHDS <b>2</b> INDUSTRIAL POSTDOCS In cooperation with Haldor Topsøe, Hempel, Dupont, Novozymes, Vølund, Rockwool International, Unibio, PHX Innovation, and Grundfos	
EDUCATION	Helps to retain, develop, and attract knowledge-based national working places, including companies with affiliates abroad.	<b>298</b> STUDENTS (STÅ**) <b>20</b> SINO-DANISH STUDENTS (STÅ**) <b>15</b> COMPLETED BENG PROJECTS <b>32</b> COMPLETED BSC PROJECTS <b>67</b> COMPLETED MSC PROJECTS	
ORGANIZATION	Attractive place to work for ambitious and technology-passionate staff members.	<b>47</b> TECHNICAL/ADMINISTRATIVE EMPLOYEES <b>98</b> PHD STUDENTS <b>95</b> SCIENTIFIC EMPLOYEES—INCLUDING 33 FACULTY	
		<hr/> <b>240</b> EMPLOYEES IN TOTAL *	
		<b>STAFF DISTRIBUTED BY AGE:</b> <b>35%</b> 20-29 <b>29%</b> 30-39 <b>14%</b> 40-49 <b>13%</b> 50-59 <b>8%</b> 60-69 <b>1%</b> 70-79	<b>FOREIGN SCIENTIFIC STAFF:</b> <b>4%</b> AFRICA <b>34%</b> ASIA <b>53%</b> EUROPE <b>5%</b> MIDDLE EAST <b>1%</b> NORTH AMERICA <b>3%</b> SOUTH AMERICA

\* 1 JANUARY - 1 DECEMBER 2016

\*\* ONE STÅ IS THE EQUIVALENT OF ONE STUDENT STUDYING FULL TIME FOR A YEAR

## CONTENTS

### ANNUAL REVIEW

**05** Welcome

### HIGHLIGHTS 2016

**08** Selected highlights of 2016

### DTU CHEMICAL ENGINEERING IN BRIEF

**12** Organization and Advisory Board

**13** Research centres and cooperating  
companies

### RESEARCH & INNOVATION

Selected feature articles from our research centres

**16** DPC  
Membrane can help patients with chronic wounds

**18** BIOENG  
Getting the best out of straw

**20** CAPEC-PROCESS  
Welcome to the world of microfluidics

**22** PILOT PLANT  
Good manufacturing practice—in practice

**24** AT CERE  
CSmall revolution may have great consequences  
for oil recovery

**26** CHEC  
CO<sub>2</sub> should be a sustainable business

**28** KT CONSORTIUM  
New cross-departmental consortium opens  
up for collaboration

### EDUCATION

**32** Programmes at DTU Chemical and  
Biochemical Engineering

**32** Courses

**34** Bachelor of Engineering degrees

**34** Bachelor of Science degrees

**34** Master of Science degrees

**35** SDC master degrees

**36** The faculty

**37** KTStudents

### PUBLICATIONS

**40** Publications

**47** Books & Monographs

**47** Contributions to books

**49** PhD theses

### USEFUL INFORMATION

**52**

Front page photo:  
Rolf H. Ringborg and Mafalda Costa Artur Dias working on a  
experimental setup for the automated kinetic characterization of  
enzymes. Photo by Thorkild Christensen





#### **Behind the process**

Frederico Montes and Carlos Eduardo Castelan behind a large stirred tank which they are using for process intensification of gas-liquid bioreactors—a core research area at the CAPEC-PROCESS Research Centre where they work as PhD-students.

Photo: Thorkild Christensen





Welcome to this Annual Report 2016 where we proudly present a small selection of our great many activities during this year within education, research, and innovation.

DTU's study programmes are becoming increasingly popular and in terms of student intake, 2016 was a year for the record books. One of the most popular branches of study was 'Chemistry and Technology', the qualifying main BSc for the MSc programmes which our department offers.

As a result, we are working hard to accommodate a reality where students not only have many different backgrounds, but also consume information in many different ways. This calls for innovative teaching methods, resulting this year in several e-learning videos that can be viewed on the digital platforms that our students use.

Innovation also goes hand in hand with research at our department. As the competition for research funds becomes fiercer, collaboration with our industrial partners accordingly becomes an important factor. Our research centres have extensive cooperation with both large global and small enterprises. It is from these relations that real innovation emerges. This year, we were proud to see that some of our innovative efforts were acknowledged with innovation awards from the Confederation of Danish Industry (DI) and at the international integrated water cycle show, iWater, in Barcelona.

Collaboration and through this, research, is further strengthened through the many conferences and annual discussion meetings that our researchers travel far to attend, as well as the ones we host ourselves. This year, we hosted 'PetroPhase 2016', the 17th International Conference on Petroleum Phase Behavior and Fouling, and we hosted the 6th international conference

on Electromechanically Active Polymer (EAP) transducers & artificial muscles. Both conferences were well-attended by industry and academia from all over the world. These meetings and conferences are important because they provide the opportunity for interchange of knowledge and thereby ensures that the research we conduct here at our department is useful to society. Adding to this, we also this year launched a cross-departmental 'KT Consortium' which we will grow to include many more relevant partners in the future. Furthermore, long-term agreements with Novozymes and Lundbeck have been extended this year, and we received the first generous grant to establish The Hempel Foundation Coatings Science and Technology Centre. Accordingly, we look forward to welcoming even more PhD students in the coming years.

The increasing number of students and research activities means that our department is growing. Just as 2016 was coming to an end, we reached an important milestone: The blueprint for our building expansion which will provide a better working environment, an improved study environment, and further development of research facilities.

I would like to close this preface by expressing my deepest gratitude to our many dedicated employees for their hard work and to thank our many national and international partners in industry and academia for sharing their knowledge and views with us. I hope you will enjoy reading about some of the many exciting results we have achieved together.

A handwritten signature in black ink, reading 'Kim Dam-Johansen'. The signature is stylized with a large, sweeping 'D' at the end.

Kim Dam-Johansen  
Professor, Head of Department









## HIGHLIGHTS

### **The first graduates from the Sino-Danish programme**

Graduation caps and dreams of the future were in the air when the very first graduates of the Sino-Danish programme in Chemical and Biochemical Engineering were celebrated at a festive ceremony in Beijing. Congratulations from DTU Chemical Engineering!

Photo: Yang Tian Peng





Photo: Ditte Valente ①



②



③

## HIGHLIGHTS 2016

### JANUARY

#### 1 January

##### PROF. RAFIQU L GANI CONTINUES AS PRESIDENT OF EFCE

After two years as President of the European Federation of Chemical Engineering (EFCE), Professor Rafiqul Gani started his second term on 1 January 2016.

##### SELF-HEALING RUBBER GOES FOR COMMERCIALIZATION

The Danish Polymer Center (DPC) received a grant from the DTU Proof-of-Concept Fund which enables researchers to get new technology ready for the market and make it possible to test it in other products. DPC aims to expand the lifespan of many often expensive products by delivering the right recipe for self-healing silicone rubber.

### FEBRUARY

#### 10,000 FOR STUDENTS GOING TO CHINA

DTU's Teknisk Kemisk Fond has established a new grant of up to DKK 10,000 to cover travel and start-up costs for Danish students who are accepted into the Chemical and Biochemical Master's programme at the Sino-Danish Center in Beijing.

#### 25 February

##### ELITEFORSK TRAVEL GRANT FOR PHD STUDENT ①

PhD Student Sofie Thage Morthensen from DTU Chemical Engineering was presented with the EliteForsk travel grant and honoured by HRH Crown Princess Mary and the (former) Danish Minister for Higher Education and Science, Esben Lunde Larsen. EliteForsk recognizes some of Denmark's most talented researchers who set the bar high and strive to be the best in their individual fields.

### MARCH

#### 31 March

##### MULTICULTURAL INSIGHTS FOR INTERNATIONAL WORK

The administrative group got to walk a day in their international colleagues' shoes in a course on 'cultural intelligence', providing insights that will strengthen the daily cooperation and understanding in the multicultural work environment that our department provides with more than 37 different nationalities.

### APRIL

#### STUDENTS EXCEL AT PETROBOWL QUALIFIERS ②

Out of more than 20 teams from student chapters within the European region, Krystian Grzegorz Klepczyk, Adam Marczyński, Hadise Baghooee, Marton L. Szanyi, and Stefano Tafliaferri ranked among the top four elite teams in the Regional Petrobowl Contest—a great achievement and so far the best ranking in the history of DTU SPE Student Chapter.

#### 26 April

##### DANISH SCIENCE FESTIVAL ③

DTU once again opened the doors to the public in order to showcase the best of science at the annual Danish Science Festival. Visitors were shown around the pilot plant, given a lecture on the history, future, and dynamics of volcanos and presented with laboratory examples of microfluidics.

#### 26 April

##### HEMPEL-DTU AWARD FOR RYBNERS HIGH SCHOOL

The Hempel DTU award was given to Rybners high school for their dedication to and encouragement of science. The award was presented by DTU Dean, Martin Vigild as part of the 'Young Scientists' finals at the 'Science in Forum' event.





Photo: Thorkild Christensen



## 29 April

### GOLD MEDAL, SAFETY PRIZE, AND SCIENTIFIC SPEECH ④ ⑤

Representation was strong at this year's DTU Commemoration Day. Professor Ole Hassager received the Julius Thomsen gold medal for excellent research throughout many years. Head of PILOT PLANT, Lars Kiørboe was honored with the Safety Prize for his long lasting dedication to help the students and employees get home safe. And, Professor Anne Meyer gave the evening's scientific speech on 'Biocatalysis for the future'.

## MAY

### 1-7 May

#### PROF. KONTOTGEORGIS APPOINTED ADJUNCT PROFESSOR

Head of AT CERE and professor Georgios Kontogeorgis visited Xi'an Jiaotong University in Xianyang, China, where he had the honour of being appointed adjunct professor to the university.

### 27 May

#### RESEARCH DAY ⑥

This year's Research Day included poster presentations and a speech on innovation by DTU's Senior Vice President for Innovation and Entrepreneurship, Marianne Thellersen. PhD student Sara Wingstrand took home the Best Research Award for her work on optimizing polymeric fibre, while the Best Innovation Award went to PhD student Arne Gladis who has developed a kinetic model to predict the mass transfer of CO<sub>2</sub> in carbon capture technology.

## JUNE

### 14-15 June

#### EAP CONFERENCE

Danish Polymer Center hosted the 6th international conference on Electromechanically Active Polymer (EAP) transducers & artificial muscles. 110 researchers from all over the world as well as several companies and research groups exhibited their knowledge about dielectric elastomer based products.

### 19-23 June

#### PETROPHASE 2016

PetroPhase 2016—The 17th International Conference on Petroleum Phase Behavior and Fouling was held in Elsinore, Denmark. The international conference was aimed at researchers in industry and academia dedicated to the study of the properties and chemistry of petroleum fluids and their effect on producing, processing, and refining in the upstream, mid-stream, and downstream industries. 180 people from all over the world attended this year's conference.

### 29 June

#### FIRST GRADUATES FROM SINO-DANISH PROGRAMME

Graduation caps and dreams of the future were in the air when the very first graduates of the Sino-Danish programme in Chemical and Biochemical Engineering were celebrated at a festive ceremony in Beijing. Congratulations to the graduates!



## HIGHLIGHTS 2016

### JULY

#### 1-30 July

##### SUMMER UNIVERSITY ⑦

While most DTU students were enjoying their holiday, the campus grounds were kept alive and kicking by Summer University participants from all around the world. 69 students came from the US universities Auburn, Case Western Reserve University, Virginia Tech, University of Alabama, Texas A&M University, and John Hopkins University. Another 5 students participated from Denmark and Portugal. 14 students from the Sino-Danish Center (SDC) also participated in the summer university course.

#### 17-25 August

##### BIOPRO WORLD TALENT CAMPUS ⑧

Solutions, socializing, and Segways. The scene for student-industry networking was set in Sorø at the annual BIOPRO World Talent Campus event, bringing together talents from all parts of the biochemical world. The Novo Nordisk Foundation was of course present as the sponsor of WTC, but also Chr. Hansen, CP Kelco, and Novozymes took part as well as the University of Copenhagen (KU-FOOD).

### SEPTEMBER

#### NEW H.C. ØRSTED POSTDOC

Marlène Vuillemin was granted a H.C. Ørsted COFUND postdoc fellowship enabled by the European Union's Marie Skłodowska-Curie actions. She will spend the next two years researching a 'Novel route to humanized glycoproteins by designed trans-sialidases (DESIGNGLYCO)'.

#### 19-23 September

##### RICHARD W. BRYERS AWARD

PhD student, Yashasvi Laxminarayan won the Richard W. Bryers award for the best student contribution at IFQ 2016 at the Czech Technical University in Prague.

#### 27 September

##### INNOVATION AWARD FOR DIGITAL WOOD STOVE

A digitally controlled wood stove with technology developed at DTU Chemical Engineering in collaboration with HWAM has won the very prestigious Confederation of Danish Industry Prize (DI Prisen).

#### 30 September

##### SCIENCE TALENTS EXPERIENCE LIFE AS SCIENTISTS

What is it like for a high school student to be a part of a high-quality technical university? The ScienceTalent Forsker camp offered 30 talented youngsters a working day in labs of DTU Chemical Engineering—encouraging them to choose the scientist's path.

### OCTOBER

#### 4-7 October 2016

##### NEW COURSE FOR INDUSTRY

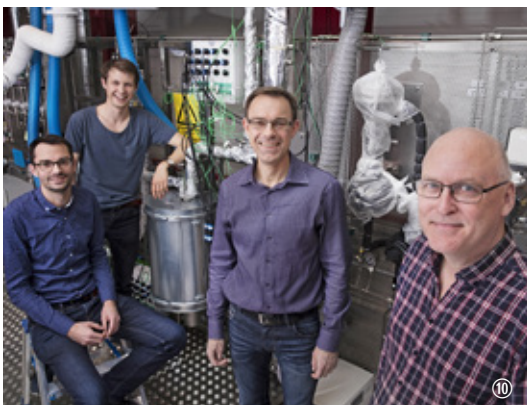
Professor Emeritus John Villadsen and Professor John Woodley gave the first course in 'Bio-process Engineering Applied to Analysis and Design of Bioprocesses'.

#### 28 October

##### ANNE LADEGAARD SKOV PHD SUPERVISOR OF THE YEAR ⑨

Champagne corks were popping at DTU's PhD reception for former students who submitted their PhD dissertation in 2016. At the celebration, Associate Professor and Head of the Danish Polymer Centre (DPC), Anne Ladegaard Skov, was presented with the honourable award PhD Supervisor of the year.





## NOVEMBER

### 9 November

#### HIGH SCHOOL INVASION

Passing on knowledge to the younger generations was at heart on 9 November. At the Danish Polymer Centre, Associate Professor Anders Egede Daugaard welcomed high school teachers into the Hempel Lab to play with polymers. In the other buildings, 63 students from Odense Tekniske Gymnasium were enjoying part of their Hempel-DTU prize: A visit to Lyngby Campus.

#### INNOVATION AWARD FOR WATINTECH PROJECT

An innovation award was given at the International Integrated Water Cycle Show in Barcelona to the inter-disciplinary project WATINTECH which covers the whole value chain around wastewater and urban run-off. Senior Researcher Xavier Flores-Alsina from CAPEC-PROCESS is in charge of WP5 (modelling and system-wide optimization).

### 30 November

#### AWARD AT DTU SUSTAIN CONFERENCE ⑩

PhD student Magnus Stummann (photo: in the back on the left) from CHEC research centre won a poster award for his work with the H2CAP project which this year succeeded in developing a new process for producing high-quality bio-fuel from beech tree.

## DECEMBER

### 4 December

#### MOVIE AWARD FOR SCIENCE CARTOONS

At the '2016 European Science TV and New Media Festival' in Lisbon the animated Microfluidics trilogy explaining the science of the two EU projects BIOINTENSE and EUROMBR won. The trilogy also won 'Best Animation Cartoon 2016' at the The Shortfest International in Malta and won silver in the Web/TV-Animation for Bleech.

#### 4X25 YEARS IN SERVICE OF THE STATE ⑪

We wish to congratulate Associate Professor Flemming Jappe Frandsen (1 Feb), Professor Anker Degn Jensen (1 Aug), Associate Professor Peter Szabo (2 Oct), and Project Manager Michael Krogsgaard Nielsen (12 Nov) on their 25-year anniversaries this year.

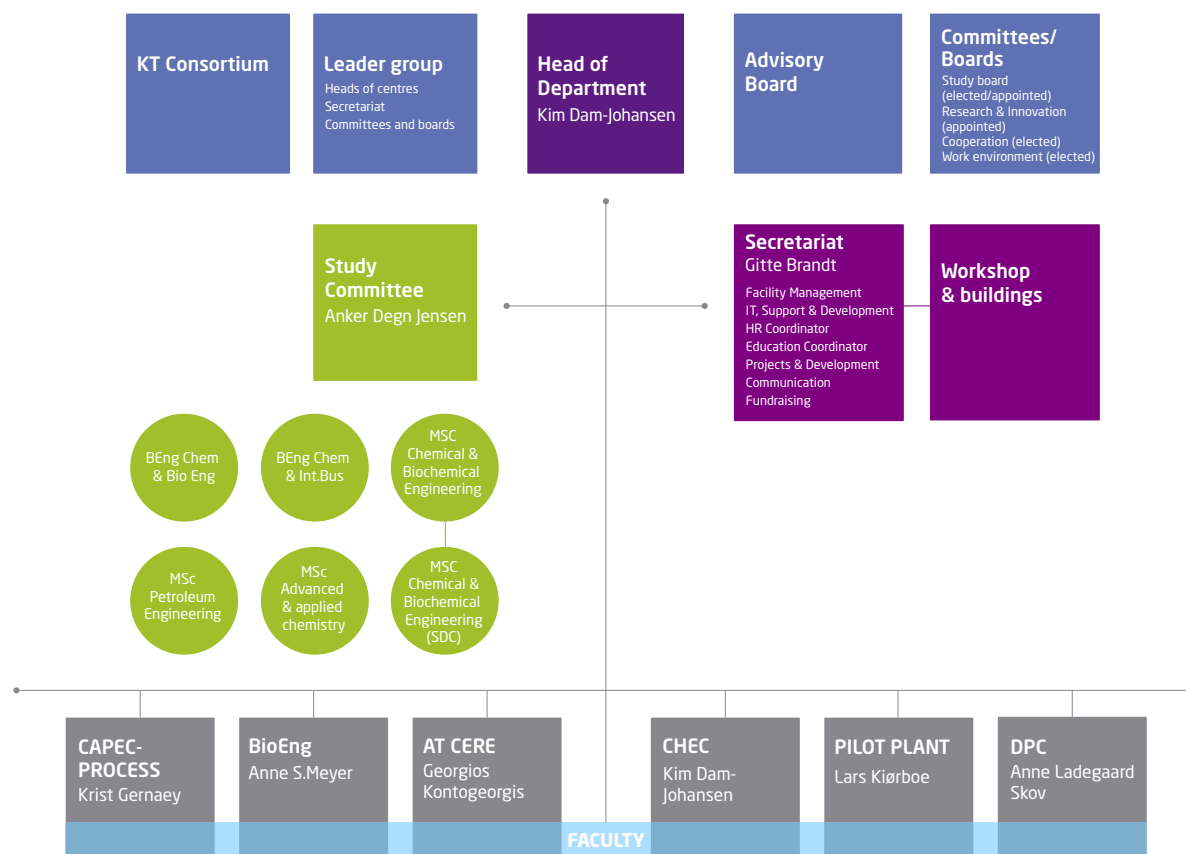
#### CONTRIBUTIONS TO OUR BOOKSHELVES THIS YEAR ⑫

This year, the book 'Fundamental Bio-Engineering'—edited by the prominent Professor Emeritus John Villadsen—finally found its way to our bookshelves. In addition, a new book on Applied Colloid and Surface Chemistry was written by Professor Georgios Kontogeorgis and Associate Professor Søren Kiil. The book is for use in our MSC course of the same name and is available on wiley.com. Professor Rafiqul Gani also co-authored the 4th Edition of the book 'Product and Process Design Principles' with professors Seider, Lewin, Widagdo and Ng. Several staff members have contributed to books which you can read about in page 47. For instance, Professor Krist Gernaey and Associate Professor Gürkan Sin contributed with a chapter on 'Data Handling and Parameter Estimation' to the book 'Experimental Methods in Wastewater Treatment'. The book has so far been downloaded more than 20,000 times—an amazing result for a technical book.

#### FIRST TWO INDUSTRIAL POSTDOCS

Innovation Fund Denmark has initiated an Industrial Postdoc programme—a collaboration between companies and research institutions about solving specific research and development tasks. This year, Seyednezamaddin Azizaddini was hired by PHX Innovation and Piotr Mazurek was hired by Grundfos.

## ORGANIZATION



## ADVISORY BOARD



**LARS BANG**

GROUP SENIOR  
VICE PRESIDENT,  
SUPPLY OPERATIONS &  
ENGINEERING,  
H. LUNDBECK A/S



**BJERNE CLAUSEN**

PRESIDENT AND CEO  
HALDOR TOPSØE A/S



**KIM PANDRUP  
CHRISTENSEN**

CHIEF TECHNICAL  
OFFICER AT ORECO A/S

"Scientific research at university level is a prerequisite for the development of Lundbeck's chemical activities in Denmark. We have had a beneficial partnership with DTU Chemical Engineering for several years, collaborating on PhD projects and recruiting several of the department's candidates. Furthermore, it has been a great advantage to be able to draw on the knowledge of DTU Chemical Engineering's scientific staff as advisors/consultants."

"Working closely with the best research groups within the fields of our core competences is of major importance to Haldor Topsoe A/S. Our cooperation with DTU Chemical Engineering enables us to resolve research challenges beyond our competences and resources and is an important source of inspiration and knowledge for employees at Haldor Topsoe, benefitting their own and the company's development."

"The close cooperation with DTU Chemical Engineering has ensured significant results in a lot of industries. Long-term focus on development and innovation is necessary to meet the ever-changing opportunities, rules, legislation, and profitability demands that all industries are faced with. DTU Chemical Engineering ensures a high level of education, motivated candidates, and industrial cooperation in important research projects that will lead to technologies of the future."



## RESEARCH CENTRES

DTU Chemical and Biochemical Engineering is home to six 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 in details, recent results, or current projects, please visit [www.kt.dtu.dk/research](http://www.kt.dtu.dk/research).

### ▶ CAPEC-PROCESS

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

### ▶ PILOT PLANT

Designing and building large-scale plants, Unit operations, Industrial chemical processes, Operational experience, Design of components, Plant safety, Good Manufacturing Practice



**Contact:**  
**Lars G. Kjørboe**  
lgk@kt.dtu.dk  
Phone +45 4525 2857

### ▶ AT CERE

Applied Thermodynamics, Transport Processes and Properties, Mathematical modeling, Material science, Petroleum Technology, Enhanced Oil Recovery, CO<sub>2</sub> capture and gas hydrates, Energy resources



**Contact: Professor**  
**Georgios Kontogeorgis**  
gk@kt.dtu.dk  
Phone: +45 4525 2859

### ▶ BIOENG

Enzyme engineering, Bioprocess enzyme technology, Biofuel production, Reactive separation technology, Biorefinery and sustainability



**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

### ▶ 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

## 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 AG  
BAWAT  
Bayer Technology Services  
BiCT  
Biofos  
BioProduct  
BP  
Calsep  
Carlsberg  
Cargill  
CelluComp  
ChemStream  
ChemProcess Technologies  
Chevron  
Chr. Hansen

CLEA  
c-LECTa  
Coloplast  
Conocophillips  
CP Kelco  
C-Tech  
Dansk Gasteknisk Center  
DHI  
DONG Energy  
DSM  
DuPont  
Esbjerg Farve- og Lakfabrik  
eCoast Marine Research  
Envidan  
Evocatall  
Evonik  
ExxonMobil  
FCC Aqualia  
FiberVisions  
Firmenich  
Fermentationexperts  
FLSmidth  
Foss  
FreeSense  
GASSCO  
GASSNOVA  
GDF-SUEZ  
GEA Process Engineering  
Gelest

Genencor  
Givaudan  
GlaxoSmithKline  
Grundfos  
H. Lundbeck  
Haldor Topsøe  
Hempel  
Hess  
HOFOR  
Hortimare  
Hwam  
Højmarks Group BHJ  
IFP  
Janssen Pharmaceutica  
KBC  
KMC  
LEAP Technology  
LEGO  
Lentikats  
Leo Pharma  
LevOss  
Lihme Protein  
Solutions  
Linde  
Lloyd's Register ODS  
Lonza AG  
Luxcel  
Maersk Oil  
MAN Diesel & Turbo

Melissa  
Meneta  
Microfluidic ChipShop  
Micronit  
Milliken  
Mitsubishi  
MOL  
Morgenfruerne  
NanomyP  
National Oilwell Varco  
Neste Jacobs Oy  
Nordic Bioenergy  
Nordic Sugar  
Nordisk Tang  
Novo Nordisk  
Novozymes  
OMV  
Ocean Rainforest  
Petrobras  
PHX Innovation  
PPG Industries  
Processium  
ProSim  
Prozomix  
Radiometer Medical  
Rambøll  
Rockwool  
RWE  
SBM Offshore

Schlumberger  
Schneider Electric  
Shell  
Sigma Aldrich  
Sika  
Sinopec  
Sintef  
Solvionic  
S-PACT  
SpinChem  
SQM  
Statoil  
Supren  
Syngenta  
Teknologisk Institut  
Tetra Pak Packaging Solutions  
Total  
Trioplast  
Unibio  
UNILEVER  
Union Engineering  
Veolia Krüger  
Wacker  
Welltec  
Xellia Pharmaceuticals








## RESEARCH & INNOVATION

### **Chalk samples**

A large part of the oil recovered in Denmark comes from underground chalk reservoirs in the Danish part of the North Sea. In the laboratories of DTU Chemical Engineering, researchers inject brines of different salinity into samples of chalk saturated with oil in order to push out the oil—a method known as ‘smart water flooding’. The progress is then monitored using X-ray computer tomography scanning.

Photo: Thorkild Christensen



Piotr Mazurek compares the sizes of two samples of the new material he has produced. The sample on the right has absorbed a lot of fluid due to its combination of silicone and glycerol. The new material could potentially be applied for many different functions in different industries—something which Mazurek is now researching as an industrial postdoc at Grundfos.

Photo: Thorkild Christensen

## ► Facts about the project

The project by Piotr Mazurek is entitled 'Glycerol-silicone elastomers as active membranes for wound dressings and beyond'.

Supervisors: Associate Professor Anne Ladegaard Skov (DTU) and Professor Michael A. Brook (McMaster University, Canada)

Objective: A list of features for an ideal chronic wound dressing has been proposed, which works as a guideline for our research. The list includes wound debridement, maintaining moist environment and gaseous exchange, absorption of blood and excess exudate, preventing infections, providing thermal insulation, low adherence, and cost-effectiveness. The aim was to create a material that would meet most (or all) these requirements and eventually create an attractive chronic wound care product.

A two-phase glycerol-silicone elastomer has been proposed as a novel membrane for wound dressings. It was discovered that this hybrid material is capable of releasing active substances when exposed to an aqueous medium. Various properties of the material (e.g. water permeability, water vapour transmission rate, water absorption, and ability to deliver active substances) were investigated and these were confronted with requirements of chronic wound treatment. Initial results are very optimistic and prove that it is possible to tune most of these properties.

Age. Obesity. Diabetes. Threats to our health that are both widespread and rising. They are also the most common causes for chronic wounds—not only painful to the patients, but often complex and expensive to treat. At DTU Chemical Engineering, a PhD project could make a difference.



# Membrane can help patients with chronic wounds

Most of us take for granted the amazing ability of our skin to heal itself. Yet, the reality for the 6.5 million patients affected by chronic wounds in the US in 2008 was quite different. At that time, it was estimated that around USD 25 billion was spent annually on treating chronic wounds. And due to the ageing population and a sharp rise in widespread diseases such as diabetes and obesity, the numbers are growing rapidly.

By mixing silicone with glycerol, former PhD student, now postdoc at the Danish Polymer Centre (DPC) Piotr Mazurek, has developed a completely new material which may solve 7 out of 8 of the issues on a recent 'wish list' for the wound dressings of the future, providing a better and more cost-efficient solution.

## Low price, high impact

Glycerol is abundant in the chemical industry and therefore very cheap. In addition to this, the methodology of mixing glycerol into silicone is quite simple and should be easy to upscale. This means that producing wound dressings in this way could be very cost-effective and therefore in high demand in a market where competition is intense.

Silicone and glycerol do not really mix; however, by spinning the ingredients at a certain rate and a certain temperature, Mazurek found that he could suspend glycerol as tiny droplets inside the silicone:

*"The more droplets I supplied, the more soft and stretchable the material got. In the end, the large number of droplets assembled like raindrops on a window creating a new structure in the material. This turned out to be very interesting indeed,"* says Piotr Mazurek.

The market already offers multiple types of chronic wound dressings and it is no news that wound dressings can release substances such as antibiotics or anaesthesia. However, Mazurek's invention goes a bit further.

## Extended treatment

According to Mazurek, the medicating dressings available in the market today, release most of the medicine rather rapidly and then the release slows down, which means a part of the medicine goes to waste and the dressing needs to be changed more often. The new material provides a longer period of medication,

which could mean more time for other care assignments for nurses and that wounds are allowed a little more time to rest. The extended release of medicine is provided by taking advantage of glycerol's ability to absorb. When the wound secretes fluids, the fluids are absorbed into the droplets of glycerol, which at the same time pushes out the medicine, creating this constant treatment effect.

## Great potential

According to Mazurek, the combination with silicone adds some more important features from the 'wish list'. Silicone has low adhesion which most people recognize from, for instance, baking moulds. It also insulates very well and protects the wound from temperature changes. Furthermore, silicone allows for gaseous exchange so that the skin to breathe while keeping a moist environment around the wound which is key to the healing process.

*"All of these properties combined in this new material gives it great potential. Not only as a wound dressing, but also for other applications. It seems like the sky's the limit and I'm excited to see what the future will bring,"* says Piotr Mazurek.



Straw is at the heart of a PhD project which earned Sofie Thage Morthensen a visit to Belgium and a rare opportunity to synthesize her own membranes.

Photo: Christian Ove Carlsson

### ► Facts

Sofie Thage Morthensen's PhD project is entitled 'Integration between enzyme technology and membrane separation in biorefinery processes', and is supervised by Associate Professor Manuel Pinelo.

The project is part of the BIOVALUE SPIR strategic platform for innovation and research on value-added products from biomass.

The objective of BIOVALUE SPIR is to ensure that Denmark is a world leader in sustainable biorefining technologies and solutions for tomorrow's bio-based society.

The Department of Chemical Engineering's Center for BioProcess Engineering leads the competences centre within Separation for BIOVALUE.

Glucose from straw may play a big role in the future production of many everyday products such as pharmaceuticals and clothes. An EliteForsk travel grant winning PhD project from DTU Chemical Engineering aims to uncover how new processes can help increase the value of straw and make it an effective and profitable business.



# Getting the best out of straw

As the world population continues to grow and the search for alternative resources intensifies, researchers are looking at different and more efficient ways to use the materials at our disposal.

Straw—a residual product from agriculture—can be used as raw material for production of, for instance, pharmaceutical products, cosmetics, and textiles. Yet, as is the case with many concepts, finances have great influence on whether or not it will become a success. Therefore, development of cost-effective processes with maximum yield and efficiency is needed. If a PhD project at DTU Chemical Engineering goes as planned, we may be one step closer to perfecting the process in the future.

## Difficult to separate

Glucose and xylose are sugars that are used to make many everyday products such as medicine and clothes. When straw is processed these sugars can be obtained, however the challenge is that glucose and xylose have very similar chemical structures and are therefore notoriously difficult to separate. A PhD project by Sofie Thage Morthensen from the Centre for Bioprocess Engineering (BioEng) could change this.

She will develop a process based on the use of membranes and enzymes in order to separate the sugar molecules in bio-refineries.

*“Membranes are super selective materials and have the potential to separate sugar molecules at a higher throughput and at milder process conditions compared to other separation processes,”* says Sofie Thage Morthensen.

The performance of the membranes can be even further enhanced with the use of enzymes as biocatalysts to modify the process stream. In scientific terms, the concept of integrating conversion and purification is known as ‘reactive membrane separation’. However, there is yet another challenge to this: Enzymes are expensive.

*“Designing processes that enable reusability and high biocatalytic productivity is a prerequisite for cost-effective enzyme use in biorefineries,”* says the PhD student.

## An EliteForsk-worthy idea

The idea has earned Sofie Thage Morthensen a travel grant from EliteForsk and she believes that travelling has given her some important experiences in working with membranes.

*“When I received the travel grant, my first priority was to go to a university where I could learn something completely new within my field. In BioEng I have only worked with commercial membranes, but at KU Leuven in Belgium I had the opportunity to synthesize my own membranes and do some more advanced characterization of them,”* says the EliteForsk grant winner.

Theory, however, is one thing. Practical application is another. Testing the reactive membrane separation on straw is the next phase of the project—and expectations are high.

*“Taking into account that most of the cost of any biorefinery process corresponds to the separation steps, membrane technology by itself has a lot to say in the development of future green processes with a more feasible exploitation of biomass. But if membrane separation is integrated with enzyme technology, the viability and simplicity of the processes can be boosted to an even higher level,”* says her supervisor Manuel Pinelo who has been researching the use of membranes for biomass conversion for around eight years at DTU Chemical Engineering.

# MICRO-FLUIDICS INSIDE



## ► Facts

BIOINTENSE is a single-stage knowledge-based bio economy (KBBE) collaborative project which started in August 2012. In collaboration with the EUROMBR project (European network for innovative MicroBioReactor application in bioprocess development) three cartoons were produced by Golderner Westen in order to disseminate the two projects to a wide audience.

The objectives of BIOINTENSE were to increase biocatalyst productivity and process intensity and thereby make way for more economically feasible processes by integration and intensification and also a shortening of the development times by developing optimized tools and protocols that can be widely applicable in industry. Furthermore, fundamental understanding on the interactions between reaction, biocatalyst and process characteristics achieved to minimize the uncertainties with respect to the cost of future biocatalytic processes. BIOINTENSE also increased understanding about the factors contributing to the total cost and environmental impact.

BIOINTENSE was EC-funded through the 7th Framework Cooperation Programme. The consortium was led by Professor John M. Woodley and manager of the project was Associate Professor Ulrich Krühne, both from the CAPEC-PROCESS research centre.

- EUROMBR is a Marie Curie initial training network (ITN). The main objective of the EUROMBR project is to deliver a trans-European network of industrially oriented specialists fully trained in the development and application of microbioreactor (MBR) technology to support the progress of innovative bio-based manufacturing processes. This project is coordinated by Ulrich Krühne and managed by Nicky Ehrlich.

A nutty professor welcomes the audience in three cartoons that were produced this year to share the otherwise complex science of the two EU projects BIOINTENSE and EUROMBR.

Watch the animated movies at:  
[www.worldofmicrofluidics.com](http://www.worldofmicrofluidics.com)

Some things are highly important, but also highly complicated. Using micro technology, the 'Mastering integration and intensification of bioprocesses' project—also known as BIOINTENSE—has yielded new, greener, and more efficient methods for future chemical production. The complex science of this project has furthermore been made available through a series of animated films that invite everyone with an interest in this promising technology into the 'World of Microfluidics'.



# Welcome to the World of Microfluidics

Food, pharma, and materials for everyday products are, more often than not, the result of several chemical processes. As such, the chemical industry is on a constant search to improve these processes to ensure that they stay competitive, remain economically attractive all the while keeping a low impact on the environment.

Traditionally, chemical processes are run on large equipment and can as a result be expensive and even harmful due to considerable waste production or use of toxic substances. One solution to avoid using such processes could be to apply enzymatic bioprocesses. In enzymatic bioprocesses enzymes from nature are used as catalysts and could in this way potentially be more productive under mild reaction conditions and yielding less waste. According to Associate Professor Ulrich Krühne from the CAPEC-PROCESS research centre, it is these bioprocess methods that need to be rethought.

*“It’s nearly impossible to reduce waste production without finding a way to distinguish the good enzymes from the bad. Here microfluidics can help us,”* says the Associate Professor who is also the project manager of the BIOINTENSE project which was concluded this year. He continues;

*“New enzymes must be designed and tested. This is the core of our project. We used a technology which first emerged in the 80’s called microfluidics. The technology enables us to control and test very small volumes of liquid and determine very precisely what works well and what does not. In this way, we can get quicker results and the small scale means we can do multiple tests at the time, making the process much more efficient”.*

## Multiple results in short time

Just like technology of microfluidics, the BIOINTENSE project has brought many results in very short period of time. New methods to increase biocatalyst productivity and process intensity through the development and application of novel microfluidic and modelling tools have been discovered. Furthermore, other points of progress include development of new microfluidic products, 24 mass fabrication compatible micro-reactors for further commercial application, standardization of device formats, making the systems applicable with standard laboratory equipment, new enzyme products and much more.

## Animating the public

There is another important side to the BIOINTENSE project. The project aimed at communicating outside of academic circles. This was done by creating the

‘World of Microfluidics’ animation films; short explanatory cartoons that have received much recognition at several science film festivals around the world. At the Shortfest International in Malta they were awarded Best Animation Cartoon 2016. At the Annual Multimedia Award they won silver for Web/TV-Animation for Bleech, and most recently they won an award at the European Science TV and New Media Festival in Lisbon. According to Ulrich Krühne, there are three main motivations for promoting the project in this way:

*“We are technical nerds here. We work in an environment where people understand our scientific lingo but of course most people are not used to this language. So communicating the project to non-technical spheres can help us with three things: Reaching young people who we will one day need to be interested in carrying on the research; making the public aware that we need to think about new and more sustainable ways to produce; and of course living up to our grant givers’ demand for communicating complex, but important science,”* says Ulrich Krühne.



Head of PILOT PLANT, Lars Kiørboe, next to a vessel connected to the CIP (Cleaning In Place) facility where students can visually experience how the plant and the process behave in real life.

Photo: Thorkild Christensen.

#### ► Main activities of the PILOT PLANT—Centre for Experimental Process and Equipment Design:

Research and teaching focused on experimental work with large-scale equipment and processes. These activities are conducted with a strong focus on industrial practice. As a result the main activities include unit operations, reaction engineering, process control, process and plant design, instrumentation, automation, and industrial measuring technology, scale-up and scale-down as well as batch versus continuous processes. New focus areas are fermentation mainly from a process point of view and particle technology.

#### ► Current projects

The project portfolio of the PILOT PLANT research centre currently includes, for instance, microbial conversion of slaughterhouse waste, syngas fermentation, and downstream processing of the liquids products, ammonia enhanced biogas production, along with fermentation experiments for the new bio-tech cluster BIOPRO and research on flowability of bulk solids and coating of particles.

#### ► Technical competences:

- Designing and building large-scale plants (engineering, construction)
- Unit operations (theory and practice)
- Industrial chemical processes (designing the entire process)
- Operational experience, solving practical process problems
- Project management
- Plant safety
- GMP (Good Manufacturing Practice)
- Wide industry contact

At DTU Chemical Engineering we have many years of experience teaching Good Manufacturing Practice or 'GMP' to students. This year, we added a continuing education course to our programme portfolio. The new GMP course has been adapted to companies in the pharma and food industry and combines theoretical aspects with practical experience using our pilot plant equipment.



# Good Manufacturing Practice —in practice

In a corner of the large pilot plant of DTU Chemical Engineering, a student is scratching his head, looking at a mobile washing station connected to a model process plant made of transparent plastic which ensures that everything going on inside is visible. A moment ago his supervisor, Lars Kiørboe, Head of the centre PILOT PLANT, pointed to a large stain of mustard stuck in one of the valves.

*“Pretend you’re standing in the big production hall of a pharmaceutical manufacturing factory. You have discovered that the CIP facility has not been able to clean the process plant entirely and every delayed second before the next batch of medicine can be produced count—what do you do?”* the experienced teacher asks.

## Practical GMP

Creating a realistic scenario tops the agenda in the Good Manufacturing Practice (GMP) courses which the centre offers to undergraduates and now also to small, medium, and large companies in Denmark. In addition to the large body of theory that goes hand in hand with the GMP world, these courses are

especially focused on practical learning aspects.

According to Lars Kiørboe, the GMP philosophy states that you cannot base the product quality on chemical analysis of the finished drug alone—GMP activities have to completely permeate the entire production process. So GMP is very comprehensive.

*“If your company is producing medicine, you cannot allow even the smallest mistake. Therefore, GMP is implemented into all steps of production from the raw material, to the design of the equipment and building, to the manufacturing processes, the education of employees further on to storage and transport of the finished products and the documentation. With our courses we want to ensure a workforce that can solve the practical challenges of GMP in the medical, food and biotech industry”* says Lars Kiørboe.

The GMP courses cover general quality standards, hygienic design, cleaning technology, documentation practice in combination with work in the pilot plant and visit to industrial sites. Since GMP is so important to large Danish companies

various aspects are also applied in other courses at the department. This includes the experimental courses in chemical unit operations where the students can work with the CIP unit and include CIP cleaning in the operation of, for instance, ultrafiltration and evaporation technologies. So the students are given a much more realistic study with experiences they can use directly in their future engineer jobs.

## Companies can test their cleaning methods

Although there are standards prescribing the best design of production equipment, the equipment will often vary from company to company and many construction details may be considered. In the pilot plant it is possible for companies to come and use our facilities for testing and developing equipment and processes, where easy changing of design and process parameters can go hand in hand with modelling and test of various raw materials. In this way, the companies can get a better understanding of the challenges they may meet and how to better solve them in the future.



Associate Professor Philip Fosbøl is pouring a sample of oil. The oil used for experiments within the SmartWater project was retrieved from two types of sedimentary rocks, chalk and greensand, which occur in the Danish part of the North Sea.

Photo: Thorkild Christensen

- ▶ Water flooding is a standard method used by oil companies all over the world in order to extract extra oil from mature fields. The 'SmartWater' project aimed to improve the theoretical understanding of the detailed mechanisms involved in water flooding and it has suggested possible ways to improve recovery rates in the Danish part of the North Sea.
- ▶ Industrial partners are Maersk Oil and DONG Energy. Funding is provided by the industry partners, by the Danish EUDP programme under the Danish Energy Agency and by the Danish research councils.
- ▶ The SmartWater project was inspired by findings in the Middle East which suggested that by modifying salinity and

What if we could get more oil from the same reservoirs? The research centre AT CERE has taken up the challenge. The SmartWater project, which was concluded this year, is an attempt to extract more oil from the available reservoirs in the Danish part of the North Sea. The methodology they have developed goes against one of the most widely held understandings in the chemistry of oil recovery.



# Small revolution may have great consequences for oil recovery

This year, the SmartWater project came to an end. Since its birth in 2011, researchers have worked hard to make oil extraction more efficient. As Philip Loldrup Fosbøl, Associate Professor at AT CERE, explains, even a small improvement could mean a big difference:

*“An oil reservoir basically consists of a big rock where the oil is embedded. Only about 30% of this oil is extracted with current conventional methods. If we could recover just 1% more oil out of the reservoirs, it would actually provide billions of DKK for the Danish State. SmartWater has been all about finding a way of doing this.”*

Yet, oil recovery is by no means a simple discipline according to the Associate Professor.

*“An oil reservoir is not a big ‘pool’ of oil somewhere under the sea floor, like many people intuitively think. It’s embedded in small holes and rooms in chalk like the kind you may remember from school. In the laboratory we use the exact same chalk combined with state-of-the-art technology to recreate the conditions*

*under which oil is extracted—all of which happens under enormous pressure. This has enabled us to find out more about the effectiveness of oil extraction without having to actually go underwater and underground”.*

## A small revolution in oil recovery

And the prospects are looking good. The project has challenged one of the basic understandings of how to best utilize the SmartWater concept. As Philip Loldrup Fosbøl says:

*“I like to think that, in the course of the project, we have revolutionized the way we think about SmartWater technology. When injecting Smartwater into the oil reservoir, small particles are formed as it mixes with the other fluids in the reservoir. Until now, scientists have believed this to be a problem, which it still is if there is too much of it and it clogs the reservoir, of course. But, what our research has also shown is that the particles are actually part of the solution: The oil ‘sticks’ to the particles and carry it to the production site. This way, we can get even more oil out,”* says the Associate Professor who has been researching oil recovery at AT

CERE for years, and believes we are now closer than ever to achieving the desired increase in oil production.

## Industry is catching on

The project has not been confined to DTU Chemical Engineering alone. DTU Civil Engineering has coordinated the project which was funded by Maersk Oil, Dong Energy and EUDP. According to Associate Professor at AT CERE, Kaj Thomsen who has been a main actor in the project, the collaboration has been of great importance and is expected to have influence on oil production in Denmark and beyond.

The new methods for oil extraction that are presented as a result of the SmartWater project have not yet been applied on a larger, industrial scale. However, this may be about to change:

*“We have a lot of ideas from the project and the industry is very interested in them—this has a lot of potential. As it looks now, one of the funders of the project will most likely try to apply the methods in the future,”* says Associate Professor, Kaj Thomsen.



Assistant Professor Jakob Munkholt next to a new piece of equipment which enables catalytic processes to be studied at a wide range of temperatures and pressures.

Photo: Thorkild Christensen

## ► Catalysis research in the CHEC research centre

The research within catalysis in CHEC focuses mainly on providing solutions to energy and environmentally related challenges, but also covers parts of green chemistry. The objectives of the research are:

To synthesize new catalytic materials

To characterize the materials using spectroscopic methods and other techniques, and by theoretical means—such as density functional theory calculations—to understand and predict the properties of the materials

To test the activity and selectivity of the materials in relevant reactions and under industrially relevant conditions, and derive kinetic models including models describing diffusion limitations applicable for real reactor design

To investigate and minimize deactivation of the catalysts under relevant conditions; To model catalytic reactors and thereby obtain an improved understanding of the interplay between the process and the catalyst

The VILLUM Center for the Science of Sustainable Fuels and Chemicals is a constellation headed by Technical University of Denmark (DTU) and with the participation of Stanford University, University of Copenhagen (KU), and the University of Southern Denmark (SDU). It is an anniversary grant on account of the 75 year of the VKR group and is the biggest grant from VILLUM FONDEN to a scientific project.

'Low-temperature processes for CO<sub>2</sub> reduction to fuels and chemical building blocks' is a project in the centre which aims to find catalysts that will work at low pressure and temperature in distributed units compatible with solar hydrogen production.

It is a very promising, but so far not entirely cost-effective process to convert CO<sub>2</sub> into useful fuels and chemicals. Developing a cost-effective process will require the right catalyst and reaction. At the CHEC research centre, researchers are developing new and more effective catalysts.



# CO<sub>2</sub> should be a sustainable business

Our planet is in need of alternative energy sources to replace fossil fuels. However, we are still far from being independent of oil, coal, and natural gases, the use of which every year leads to tons of CO<sub>2</sub> being emitted into the Earth's atmosphere. But what if you could use this otherwise harmful greenhouse gas for storing green energy or producing useful chemicals for everyday products? Around the world, researchers are racing to find an effective and affordable way to achieve exactly this. And, according to Anker Degn Jensen, Professor at DTU Chemical Engineering, CO<sub>2</sub> could very well become an important resource in the future.

*"Almost all fuels and chemicals contain carbon which today is obtained from fossil fuels. However, CO<sub>2</sub> is also a possible source of carbon. So, when we no longer wish to use or do not have any more fossil fuels, the ability to effectively convert CO<sub>2</sub> into chemicals could prove to hold great potential in the long run. And in the meantime, large point sources – such as power plants and cement factories – are attractive sources of CO<sub>2</sub>," says the professor and catalysis expert.*

Methods to convert CO<sub>2</sub> into, for instance, ethanol – one of the promising alternatives to fossil fuels – already exist. However, there is a significant bump on the road: The process remains too

ineffective and the yield of ethanol too low in the end. Therefore, Professor Anker Degn Jensen together with his colleague from the CHEC research centre, Assistant Professor Jakob Munkholt, are working with colleagues from DTU and Stanford University to find a solution that is both environmentally and economically attractive. Their research project is called 'Thermally driven processes for CO<sub>2</sub> reduction to fuels and chemical building blocks'. The aim of the project is to develop a catalyst which can convert CO<sub>2</sub> into ethanol at a low pressure and temperature. Conversion of CO<sub>2</sub> traditionally requires a great amount of energy. However, if it can be done at lower pressures and temperatures, it will be feasible to use, for instance, solar or wind power for the process. The ethanol can, as such, become a way to store the electricity produced from these sustainable energy sources.

## Too much is wasted

Ethanol can be produced by a reaction between CO<sub>2</sub> and hydrogen using a catalyst. However, the challenge with this process is that the currently best catalysts used for this reaction cannot prevent that a significant part of the CO<sub>2</sub> ends up as unwanted light hydrocarbons, particularly methane. Furthermore, too much of the hydrogen is wasted as it is converted into water.

*"The waste of hydrogen is problematic, as there are significant costs associated with producing hydrogen and that means we are still relatively far from having anything of commercial interest. That's why we are trying to develop new catalysts with the ability to effectively convert CO<sub>2</sub> into ethanol as well as other valuable alcohols to replace fossil fuels," says Assistant Professor Jakob Munkholt Christensen.*

## Difficult, but with great potential

Although converting CO<sub>2</sub> is a challenging process, the team of researchers are optimistic about finding the right materials with the right abilities to make effective catalysts.

*"Rhodium-based catalysts have shown great potential, but are expensive. We will research how and why it functions so well and with this knowledge we hope to imitate the properties to make a cheaper synthetic catalyst," says Jakob Munkholt Christensen.*

The project is part of the new V-Sustain research centre at DTU focusing on sustainable chemicals and fuels. The work was kicked off in the summer of 2016 and will continue for the next eight years with four new PhD students expected to be hired at DTU Chemical Engineering.



Here are the people behind the new KT Consortium. So far the consortium counts ten PhD students, a postdoc, a research assistant, a secretary along with associated faculty members—and not least—17 member companies from all over the world.

Photo: Thorkild Christensen

## ► Facts about the KT Consortium

The consortium was established in 1997 by Professors Rafiqul Gani and Sten Bay Jørgensen under the name CAPEC consortium.

Currently, the KT Consortium offers:

### **Computational tools**

Property estimation methods, mathematical models, numerical solvers, process simulators, process-product synthesis/design toolbox, process control toolbox, and many more.

### **Technology**

Methodologies for process-product synthesis, design, analysis and control/operation, simulation strategies, solvent selection/design, pollution prevention, sustainable process-product alternatives and many more.

### **Application**

Industrial case studies, tutorial case studies, technology transfer studies, and consulting.

The former CAPEC consortium has been reorganized into a united cross-departmental consortium called KT Consortium. Masterminds behind the consortium are Head of Department Professor Kim Dam-Johansen and Professor Rafiqul Gani who with this strategic move will strive to take the department's collaboration with industry partners to the next level—a networking platform in full scale.



# New cross-departmental consortium opens up for collaboration

KT Consortium is an industry-academia collaboration that offers networking opportunities, state-of-the-art methods, and tools to its members in the chemical, petrochemical, pharmaceutical, agrochemical, food and biochemical industries.

*"KT is short for KemiTeknik, the Danish version of our name,"* Kim Dam-Johansen explained at the opening of the very first KT Consortium Annual Meeting at DTU on 28 October 2016.

The consortium will continue to develop generic methods and tools using computer aided systems approach to solve and analyse problems related to product-process modelling, simulation, synthesis, design, analysis, control, and operation in collaboration with the member companies. Yet, these services are going to be broadened in the future according to Kim Dam-Johansen.

*"The name is new, so are the future perspectives. Although the consortium originally was established in 1997, this is not a case of old wine in a new bottle,"* says Kim Dam-Johansen about the recent developments.

*"In the future, research from all our six research centres will be included and more industrial partners from both small, medium and large enterprises from all over the world will be invited to join. My hope is that this broader mix of knowledge and experience will strengthen our ability to deliver directly applicable research that solve the future challenges of our global society,"* he explains.

## Going far for innovation

Present at the KT Consortium Annual Meeting was Graduate Programme Lead, Manufacturing at GlaxoSmith-Kline, Dr Conchita Jimenez-Gonzalez. Coming all the way from the US, there must be some good reasons to join the annual meetings according to Dr Jimenez-Gonzalez, who has been a frequent visitor since 2003 when Glaxo-SmithKline became a member.

*"Always before I come here, I do a good amount of research and I always find good things on the agenda,"* says Dr Jimenez-Gonzalez and continues, *"I like that I get updated on developments in the research arena. I like the opportunity to be in some projects. And now that I'm leading the graduate programme in my company, I've brought six of my UK grad-*

*uates to this meeting. I'm really interested in hopefully providing them with a view of the world of research besides what we do at the company, because I do believe that the more people are exposed to different research, the better their work is and the more innovative their thoughts become".*

As Programme Lead, Conchita Jimenez-Gonzalez believes a good chemical engineer is a problem solving professional that is really good at thinking in networks, because nothing happens in isolation.

*"It might be that there is a tool that we can't use right away in the company, but it might spark another idea of something else that we can use. That's always, I think, how innovation works, it's not just somebody sitting alone in a room. It's the cross-pollination of ideas,"* says Conchita Jimenez-Gonzalez.

## Open for new members

The KT Consortium is open for new company members. Read about the new consortium, services and how to apply for membership on the website [www.kt.dtu.dk/research/kt-consortium](http://www.kt.dtu.dk/research/kt-consortium).







## EDUCATION

### Polymers and particles

Synthesis of polymers (flask) and surface modification of particles (small vials) can be used to control agglomeration of particles (petri dish).

Photo: Thorkild Christensen

# Programmes at DTU Chemical and Biochemical Engineering

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 disci-

plines 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, computer modelling, process and product design.

---

## COURSES 1 SEPTEMBER 2015 – 31 AUGUST 2016

### PHD COURSES

28901	Advanced Computer Aided Modelling
28902	Process & Tools Integration
28904	Soft Matter 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
28923	Uncertainty and Sensitivity Analysis of Numerical Models
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 2016, with the number of students attending shown in brackets. Courses for Bachelor of Engineering 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 (55) (B)
28016	Mathematical models for chemical and biochemical systems (72) (B)
28017	Chemical and Biochemical Process Engineering (21) (B)
28020	Introduction to Chemical and Biochemical Engineering (63)
28022	Unit Operations of Chemical Engineering and Biotechnology (87) (B)
28025	Bio Process Technology (83)
28121	Chemical Unit Operations Laboratory (10)
28122	Chemical Unit Operations Laboratory—3 weeks Summer University Laboratory (7)
28124	Summer course in chemical process and plant design (14)
28157	Process Design (40) (B)
28160	Mathematical models for chemical systems (45)
28212	Polymer Chemistry (15)
28214	Polymer Synthesis and Characterization (7)
28221	Chemical Engineering Thermodynamics (31)
28231	Laboratory in Chemical and Biochemical Engineering (18)
28322	Chemical Engineering Thermodynamics (61) (B)
28342	Chemical Reaction Engineering (53) (B)
28344	Biotechnology and process design (64) (B)
28345	Chemical Reaction Engineering (34)
28350	Process Design: Principles and Methods (47)
28352	Chemical Process Control (40) (B)
28361	Chemical Engineering Model Analysis (20)
28415	Oil and Gas Production (45)
28423	Phase Equilibria for Separation Processes (20)
28434	Membrane Technology (40)
28443	Industrial Reaction Engineering (33)
28451	Optimizing Plantwide Control (17)
28811	Polymers in Processes and Products (5)
28850	Quality by Design (QbD): Integration of product and process development (64)
28855	Good Manufacturing Practice (60)
28864	Introduction to Matlab Programming (26)
28871	Production of Biofuels (15)
28885	Technology and Economy of Oil and Gas Production (49) (B)

#### Courses offered together with other departments:

26317	Instrumental Chemical Analysis (33)
27944	Biotechnology and process design (11) (B)
41683	Materials Science (70) (B)

### FALL SEMESTER

228001	Introduction to Chemistry and Chemical Engineering (67)
28012	Chemical and Biochemical Process Engineering (72) (B)
28016	Mathematical models for chemical and biochemical systems (89) (B)
28022	Unit Operations of Chemical Engineering and Biotechnology (86) (B)
28121	Chemical Unit Operations Laboratory (18)
28125	Chemical Unit Operations Laboratory (24)
28140	Introduction to Chemical Reaction Engineering (39)
28150	Introduction to Process Control (66)
28157	Process and product design (37) (B)
28213	Polymer Technology (55)
28233	Recovery and Purification of Biological Products (55)
28242	Chemical Kinetics and Catalysis (51)
28244	Combustion and High Temperature Process (55)
28246	Applied Enzyme Technology and Kinetics (55)
28247	Advanced Enzyme Technology (15)
28310	Chemical and Biochemical Product Design (51)
28315	Colloid and Surface Chemistry (63)
28316	Laboratory Course in Colloid and Surface Chemistry (19)
28322	Chemical Engineering Thermodynamics (78) (B)
28342	Chemical Reaction Engineering (34) (B)
28352	Chemical Process Control (32) (B)
28361	Chemical Engineering Model Analysis (56)
28420	Separation Processes (39)
28515	Enhanced Oil Recovery (42)
28530	Transport Processes (60)
28831	Computational fluid dynamics in chemical engineering (23)
28845	Chemical Reaction Engineering Laboratory (22)
28852	Risk Assessment in Chemical Industry (26)
28864	Introduction to Matlab Programming (31)
28870	Energy and Sustainability (127)
28872	Biorefinery (49)

#### Courses offered together with other departments:

23522	Rheology of food and biological materials (10)
26010	Introductory Project in Chemistry (49)
27004	Health, Diseases and Technology (68)
27944	Biotechnology and process design (30) (B)
41683	Materials Science (35) (B)

## BACHELOR OF ENGINEERING DEGREES

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

Agertoft, Frederik Cornali	Technical and economical evaluation of using a radial flow methanol converter as part of the reactor capacity in a methanol synthesis loop
Ali, Nabila Nasrudin Abdulqadir	Yield of Insulin aspart in purification
Alwan, Zaman Mothana	Removal of selenium from waste water
Al-Asfar, Ali Omar	Investigation of a rotational pumping element
Appelt, Julius Lai & Struve, Rasmus	Investigation of the properties of ceria-zirconia mixed oxide catalysts for systems removing particulates and Nox from diesel vehicle exhaust
Azizi, Haroon-Ur-Rashid	Cyclic separation
Cakir, Meral	Re-installation of utility-plant: Liquid waste handling and water circulation line
Carlsen, Niels Frahm Vilhelmsen	Technoeconomic analysis of a glycerol processing plant with forward osmosis for water recirculation
Jepsen, Ulf	Simulation of absorption heat pump for flue gas condensation
Kurlink, Kristian Wismann	Effect of adhesives on noise damping
Laczek, Kim	Processes for the separation of rare earth elements from ores
Larsen, Gudrun F. Gudmundsdottir	Modelling of carboxylic acid extraction from fermentation broth
Nærum, Nicolai Peter	Systematic synthesis of a methyl acetate production plant
Pallesen, Jeppe Væver	Stability measurement and equilibrium modelling of ozonated edible oils for medical treatments

## BACHELOR OF SCIENCE DEGREES

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

Andersen, Bastian Borum	Model Development for Cyclic Distillation
Andersen, Jakob Afzal	Removal of particulates and NOx from automotive exhaust gas by combined diesel particulate filter and SCR
Andersen, Mads Gade	Dynamic Simulation Study of Falling Film Evaporation
Biel-Nielsen, Tessa Lund	Measurement and Modeling of Gas Diffusion in Coated Enzyme Particles
Bokhari, Syed Muhammad Qasim	Reaction Equilibria in Liquids
Boye, August	Mechanism for Fouling of Waste Heat Boiler Tubes in Regeneration of Spent Sulfuric Acid
Brogaard, Mads Schack	The Influence of the Operating Conditions and Influent Composition on the Reactor Performance in a Full-Scale "Anaerobic
Bugge, Anders	Solvent Exchange in Continuous Processing
Fayyaz, Umar	Recycling of Phosphorus From Biomass Ashes
Freiesleben, Louise la Cour	Commissioning of Fluidized Bed Coating Equipment
Gong, Wentao	Modeling the Aqueous Acetic Acid-Sodium Acetate-Potassium Acetate System
Hambartsumyan, David Sargis	Screening of resins with improved binding capacity of Vancomycin under static and dynamic conditions
Hansen, Michael Kolling	Proactive Well Workover Maintenance Model
Jacobsen, Bjartur	Rate-Based Model for Enzyme Upgrading of Biogas
Jensen, Martin Pilgaard	Combustion Behavior of Bio Slurry Oils and Their Use in Boilers
Johansen, Mathias	Advanced Control Strategies for N2O Control From Wwtps
Jørgensen, Sigurd Bay	Studies of the Active Site and Reaction Mechanism for the Industrial Methanol Synthesis Catalyst
Kjeldbjerg, Camilla Maria	Heat Transfer in Dielectric Elastomers and its Influence on Dielectric Breakdown
Kreutzfeldt, Mads Grøndal	Techno-Economic Study of Carbon Dioxide Capture and Conversion
Li, Jiangui	Measurement and Correlation of Kinetic Rate Constants in Enzymatic Promoted CO2 Removal Solvents
Lomholdt, Niels Frithjof	Pilot scale Development, Measurements and Modelling of Enzyme Catalysed CO2 Removal Processes
Nguyen, Thanh Thien	Synthesis and Quantification of Various New Poly(acrylate)/PDMS Interpenetrating Networks
Nielsen, Rasmus Fjordbak	Design of Cyclic Distillation Units
Olsen, Martin Due	Modeling of Phase Equilibria for Salt-Acetone-Water Mixtures
Pol, Isabel	Conversion of Lignosulfonate to Value-Added Chemicals
Rasmussen, Jess Bjørn	HCl Absorption by Raw Meal
Rehman, Mujeeb Ur	Recycling of Phosphorus From Biomass Ashes
Schmidt, Morten Saaby	Degradation of Keratin by Bacteria
Sieverts, Michael Gram	Methods of permeability measurements
Sode, Michael	Catalytic oxidation of methane
Tomás, Elena	Conversion of Lignosulfonate to Value-Added Chemicals
Zilstorff, Frederikke Byrial	Experimental Determination of the Solubility of Exotic Scales at High Pressures and High Temperatures

## MASTER OF SCIENCE DEGREES

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

Abdullahi, Abdirahman	Separation of trace components from aqueous solution
Aloupis, Georgios	Modelling of thermodynamics of hydrate inhibitor systems
Andersen, Christian	Preparation of bio-based polymers by enzymatic polymerization
Andreassen, David Richterhausen	Reduction of Metal Contaminants in Coal Tars
Assaf, Rima Adnan	Identification of antioxidants in polymers by HPLC
Baghooee, Hadise	Propagation of the liquid-liquid interface in a two-phase flow in a porous medium
Berendt, Kasper Leonhard	Enzyme immobilization on ceramic membranes
Bisgaard, Jonas	Development and use of sensor particles
Bonde, Christian Loft	Speciation of Chemistry in Biomass Ashes
Bloch, Cæcilie Sejr	Optimal catalyst composition for a propane dehydrogenation catalyst
Calvera, Cristina Plaza	Sustainable CO2 Capture and Conversion Process Design
Camacho Vergara, Edgar Luis	Modelling Gas Hydrates with Improved Langmuir Adsorption constants



## MASTER OF SCIENCE DEGREES

Chatterjee, Rishika	Studies of the Interaction between Cu and ZnO in the Industrial type Methanol Catalyst
da Costa Martins, Duarte Miguel	Study of Vitamin Stability
Dias Freitas de Lima O. Marlene Alice	Development and use of sensor particles
Gadeberg, Matias Normann	Development of model predictive control for falling film evaporators
Garg, Nipun	Fines formation during CO <sub>2</sub> low salinity WAG (CO <sub>2</sub> LSWAG) EOR
Gonzalez Garcia, Marta	Solvent Based Separation of Azeotropic Mixtures
Gottschalck-Andersen, Jacob Rom	Modelling of drying and its effects on catalytic activity
Gupta, Shivangi	Long-term durability of silicone coatings for biofouling protection of ships
Hansen, Martin Møller	Upscaling of catalytic fixed bed reactors
Hao, Jiazheng	Experimental study of enhanced oil recovery by application of advanced chemicals
Højgaard, Lise Bomholt	Emergency assessment of aspects related to conversion of seaweed into value-added products in Ghana
Israelsen, Kasper Christian	Development of a glucose oxidase method for mass transfer characterization in a bioreactor
Jhamb, Spardha Virendra	Development of a Model for Ultrafiltration Systems
Karlsen, Kristian Barreth	Seaweed fingerprinting and bioprocessing
Kepa, Katarzyna	Grafting on ionic monomers onto ePTFE for improvement of facial implants
Khusainov, Ilmur	Diffusion in Protective Organic Thermoset Coatings
Kikas, Erki	Simulation and Analysis of a Deodorization Process
Kurz, Dorothee Luise	Microbial diversity in a fast anaerobic biofilm digestion biogas system
Latipov, Rifnur	Characterization of PEO-based copolymers' behaviour and stability in fouling-release coatings
Leth-Espensen, Anna	Mathematical Modeling of Coffee Extraction in Packed Beds
Lodberg, Anders	Modeling and experiments for recycling of phosphorus
Lundquist, Casper Wolf	Improved dissolved oxygen control in fermentations with filamentous fungi
Lydom, Simon Ingvar	Emissions from Cement Production
Lymperis, Konstantinos	Modeling H <sub>2</sub> S and COS balances in underground natural gas storage facilities
Madsen, Line Riis	The effect of entrapped air on drying droplets in a spray dryer
Malek-Shah, Masoud Mohamed	Validation of a general acid-base equilibria model plug-in for bio-based processes
Marke, Henrik Sander	Modeling of a microfiltration recovery process
Marques Couto, Rita Margarida	Accessory enzymes for improved removal of carbohydrates from biorefinery lignin
Masik, Joosep	Modeling Oxygen Mass Transfer in a Static Mixer Section of a U-Loop Reactor
Meester, Michel	Influence of additives on soot formation in diffusion flames
Meyer, Kristian	Simulation tool development and control study of heat integrated distillation
Milla Diaz, Kevin Julio	Simulation of enzyme-based biogas upgrading
Mortensen, Søren	Further development of the electrolyte equation of state for electrolyte systems
Mosbech, Caroline	Genom-based enzyme discovery
Muse, Mohamud Abdi	Simulation of Heat pump for flue gas from wood chip combustion
Neerup, Randi	Kinetics of enzyme-enhanced CO <sub>2</sub> capture
Nemming, Louise Kjer	Biogas production in fixed filter fixed film reactor systems
Nielsen, Mette Joan	Concentration of liquid from pre-treated sugar beets by using membrane technology
Nielsen, Nans Liv	Substrate selectivity of endo-beta 1,4-mannanases
Palazon, Lorena Bianco	Continuous production of solvent-based coatings
Paraskeva, Ioulietta	Solvent Swap Method for Separation Tasks
Pedersen, Patrick Nicklas	NO <sub>x</sub> in RDF combustion
Pronk, Robin Christiaan	Experimental study of clay fines migration as a consequence of low-salinity water injection
Rajendram, Rajatheepan	Solubility modeling of active species
Rasmussen, Morten Lund	Thermal conversion of CH <sub>3</sub> Cl
Rodriguez Pupo, Alejandro	Thermodynamic modeling of scale formation in brines from HP/HT reservoirs
Rosanas, Ana-Sofia Sanchez Arcilla	Superstructure based Optimization for Synthesis of Biofuels and Chemical Processing Routes
Sayed, Abdullah Mohammad	Design and process for the removal of SO <sub>2</sub> from diesel exhaust
Schmidt, Ricky Daniel	Polymeric materials for medical applications
Schouw, Mathias	Development of gasoline isomerization kinetics and study of carbon compounds deposited on the catalysts used in the upgrading of TIGAS gasoline
Seaby, Brian Graham	Value-added biochemical production from complex substrates
Sigurdardóttir, Sigyn Björk	A membrane bioreactor for high performance production of fluconic acid and lactic acid
Svith, Casper Stryhn	Single particle modeling of RDF combustion
Toderascu, Andreea Genoveva	Kinetics for gasification of biomass char
Torbensen, Kasper	Proactive well workover & maintenance model

## SDC MASTER DEGREES

14 students completed their research projects for the MSc degree/dual degree. The project titles and names of the students are listed below:

Cao, Xiaotong	The preparation and application of a multifunctional membrane based on polydopamine (PDA) coatings
Chen, Yuan	Co-production of activated carbon, bio-oil and combustible gases from pyrolysis of penicillin mycelial dreg
Feng, Kai	Stability of bioreactors responding to environmental disturbance associated with microbial diversity
Fu, Zhaolin	In-situ hydrodeoxygenation upgrading of bio-oil
Ge, Yuanzheng	System Evaluation of Power To Gas
Ni, Lingli	Synthesis of terephthalic acid from cellulose derivatives
Qi, Chunping	Recycle of TiO <sub>2</sub> carrier from Waste SCR catalyst and property evaluation of fresh SCR catalyst made by this recycled carrier
Shan, Youna	Cellulose-based hybrid aerogels
Song, Yuanmei	Promotion of methane hydrate formation by adding other trace of gases
Tian, Tian	Validation study on the continuum modeling of dense granular flow
Wang, Xingxing	Synthesis of diphenyl carbonate from phenol and carbon dioxide catalyzed by multi-functionalized ionic liquid
Yao, Haoyu	Removal of nitrogen-containing compounds from fuel oil through reactive extraction
Zhang, Jingyuan	CFD simulation of an industrial MTO fluidized bed reactor
Zhang, Yaqin	Computational study of dissolution of lignin in ionic liquids

# THE FACULTY 2016

## SCIENTIFIC



Jens Abildskov  
Associate Professor



Jakob Munkholt  
Christensen  
Assistant Professor



Karsten H. Clement  
Professor (Docent)



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



Anker D. Jensen  
Professor



Søren Kiil  
Associate Professor



Georgios M.  
Kontogeorgis  
Professor



Ulrich Krühne  
Associate Professor



Xiangdong Liang  
Assistant Professor



Anne 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 Hundedøl  
Special Consultant,  
PILOT PLANT



Lars Klørboe  
Head of PILOT PLANT



Søren Hvilsted  
Professor  
(Research manager)



Gunnar Jonsson  
Associate Professor  
Emeritus



Sten Bay Jørgensen  
Professor Emeritus



Michael L. Michelsen  
Professor Emeritus  
(Docent)



John Villadsen  
Professor Emeritus

## 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 the top-left row: Joachim Thrane, Parth Joshi, Nail Tamaev from the left bottom row: Christian Schandel, Hugo Mobarec, Kristian Krum (missing from the photo: Andres Pelayo)  
Photo by: Christian 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 and Biochemical Engineering to generate awareness about the research centres and to facilitate a direction for BSc, MSc or PhD thesis topics.

## GUESTS

### VISITING PHD STUDENTS

**Yang Wang** from North China Electric Power University, China  
**Miguel Àngel Vázquez Domínguez** from Dept. de Ingeniería Química y Ambiental, Spain  
**He Liu** from Chinese Academy of Sciences, China  
**Xiaolong Li** from University of Petroleum, China  
**Isabel Maria Gonzalez Delgado** from URJC, Spain  
**Seongwoong Bae** from KAIST, South Korea  
**Shuai Yang** from University of Chinese Academy of Sciences, China  
**Shiwen Sun** from TU Graz, Austria  
**Maximilian Kuhnhen** from TU, Darmstadt, Germany  
**Anna Panteli** from Imperial College London, UK  
**Salvatore Constanzo** from University of Kreta, Greece  
**Xianling Zheng** from Institute of Bioenergy & bioprocess Technology, China  
**Shi Huang** from Qingdao Institute of BioEnergy & Bioprocess Technology, China  
**Aurora Srishti** from University Montpellier, France  
**Alessandro Rosengart** from Politecnico de Milano, Italy  
**Boeun Kim** from KAIST, South Korea  
**Dasom Lm** from KAIST, South Korea  
**Klaus Pellicer Alborch** from TU, Berlin, Germany  
**Matej Danko Slovak** from University of Technology, Bratislava, Slovakia  
**Stefano Lillia** from Politecnico de Milano, Italy

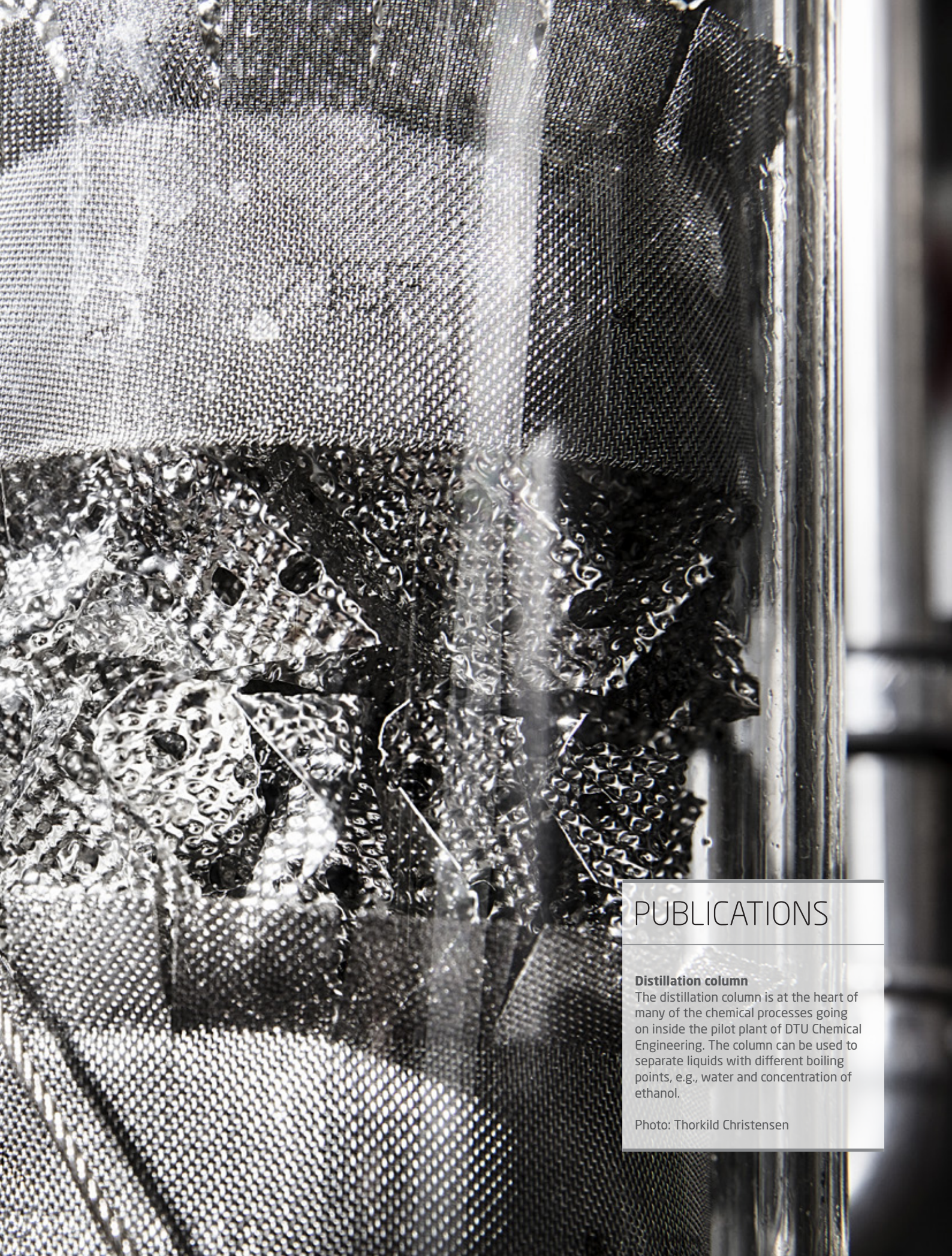
**Teng Ma** from Chinese Academy of Sciences, Beijing, China  
**Xinsheng Hu** from China University of Mining & Technology, China  
**Huang Shi** from QIBEBT, Chinese Academy of Science, China

### OTHER VISITORS

**Postdoc Xiaoguang Yang** from Harbin Eng. University, China  
**Professor Luke E.K. Achenie** from Virginia Tech., USA  
**Professor Victor M. Ugaz** from Texas A&M University, USA  
**Professor Karim Muhammad Nazmul** from Texas A&M University, USA  
**Professor John Kim** from University of Alabama, USA  
**Professor Paul Marchall** from University of North Texas, USA  
**Professor Bernhard Hauer** from University of Stuttgart, Germany  
**Professor Heath Turner** from University of Alabama, USA  
**Professor Michael A. Brook** McMaster University, Canada  
**Professor Dimitrios Vlassopoulos** from University of Crete, Greece  
**Professor Yujun Wang** from Tsinghua University, China  
**Professor Zhimin Lu** from South China University of Technology, China  
**Assistant Engineer Megane Richez** from Polytech Grenoble, France  
**Engineer Julian Le** from INSA Lyon, France  
**Senior researcher Dou Kejun** from CNREC, China  
**Researcher Jisong Bai** from Chongqing University of Science & Technology, China







## PUBLICATIONS

### **Distillation column**

The distillation column is at the heart of many of the chemical processes going on inside the pilot plant of DTU Chemical Engineering. The column can be used to separate liquids with different boiling points, e.g., water and concentration of ethanol.

Photo: Thorkild Christensen



- Aili, David; Javakhishvili, Irakli; Han, Junyoung; Jankova Atanasova, Katja ; Pan, Chao; Hvilsted, Søren; Jensen, Jens Oluf; Bjerrum, Niels J.; Li, Qingfeng / **Amino-Functional Polybenzimidazole Blends with Enhanced Phosphoric Acid Mediated Proton Conductivity as Fuel Cell Electrolytes**. *Macromolecular Chemistry and Physics*, Vol. 217, No. 10, 2016, pp. 1161-1168.
- Ale, Marcel Tutor; Barrett, Kristian; Addico, Gloria; Rhein-Knudsen, Nanna; deGraft-Johnson, Amoako; Meyer, Anne S. / **DNA-Based Identification and Chemical Characteristics of *Hypnea musciformis* from Coastal Sites in Ghana**. *Diversity and Distributions*, Vol. 8, No. 2, 2016.
- Anantpinijwatna, Amata; Kim, Sun H.; Sales-Cruz, Mauricio; O'Connell, John P.; Gani, Rafiqul / **Application of the e-KT-UNIFAC Model for the Improved and Innovative Design of Biphasic Reacting Systems**. *Journal of Chemical & Engineering Data*, Vol. 61, No. 12, 2016, pp. 4090-4103.
- Anantpinijwatna, Amata; Sales-Cruz, Mauricio; Hyung Kim, Sun ; O'Connell, John P.; Gani, Rafiqul / **A Systematic Modelling Framework for Phase Transfer Catalyst Systems**. *Chemical Engineering Research & Design*, Vol. 115, No. Part B, 2016, pp. 407-422.
- Andersen, Nina Marianne; Cognet, T.; Santacoloma, pp. 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.
- Arrad, Mouad; Kaddami, Mohammed; Goundali, Bahija El; Thomsen, Kaj / **Solubility Modeling of the Binary Systems  $\text{Fe}(\text{NO}_3)_3\text{-H}_2\text{O}$ ,  $\text{Co}(\text{NO}_3)_2\text{-H}_2\text{O}$  and the Ternary System  $\text{Fe}(\text{NO}_3)_3\text{-Co}(\text{NO}_3)_2\text{-H}_2\text{O}$  with the Extended Universal Quasichemical (UNIQUAC) Model**. *Journal of Solution Chemistry*, Vol. 45, No. 4, 2016, pp. 534-545.
- Arya, Alay; Liang, Xiaodong; von Solms, Nicolas; Kontogeorgis, Georgios / **Modeling of Asphaltene Onset Precipitation Conditions with Cubic Plus Association (CPA) and Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) Equations of State**. *Energy & Fuels*, Vol. 30, No. 8, 2016, pp. 6835-6852.
- Awan, Javeed A.; Coquelet, Christophe; Tsivintzelis, Ioannis; Kontogeorgis, Georgios / **Phase Equilibrium Measurements and Modelling of 1-Propanethiol+1-Butanethiol +  $\text{CH}_4$  in Methane Ternary System at 303, 336, and 368 K and Pressure Up to 9 MPa**. *Journal of Chemical and Engineering Data*, Vol. 61, No. 1, 2016, pp. 41-44.
- Banik, Sindrita Dutta; Nordblad, Mathias; Woodley, John; Peters, Günther H.J. / **A Correlation between the Activity of *Candida antarctica* Lipase B and Differences in Binding Free Energies of Organic Solvent and Substrate**. *ACS Catalysis*, Vol. 6, No. 10, 2016, pp. 6350-6361.
- Bataillon, Thomas; Galtier, Nicolas; Bernard, Aurelien; Cryer, Nicolai; Faivre, Nicolas; Santoni, Sylvain; Severac, Dany; Mikkelsen, Teis Nørgaard; Larsen, Klaus S.; Beier, Claus; Sørensen, Jesper G.; Holmstrup, Martin; Ehlers, Bodil K. / **A replicated climate change field experiment reveals rapid evolutionary response in an ecologically important soil invertebrate**. *Global Change Biology*, Vol. 22, No. 7, 2016, pp. 2370-2379.
- 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*, 2016.
- Baum, Andreas; Hansen, pp. W.; Nørgaard, Lars; Sørensen, John; Mikkelsen, Jørn Dalgaard / **Rapid quantification of casein in skim milk using Fourier transform infrared spectroscopy, enzymatic perturbation, and multiway partial least squares: Monitoring chymosin at work**. *Journal of Dairy Science*, Vol. 99, No. 8, 2016, pp. 6071-9.
- Bîldea, Costin Sorin; Pătruț, Cătălin; Jørgensen, Sten Bay; Abildskov, Jens; Kiss, Anton A. / **Cyclic distillation technology—A mini-review**. *Journal of Chemical Technology and Biotechnology*, Vol. 91, 2016, pp. 1215-1223.
- Bisgaard, Thomas; Skogestad, Sigurd; Abildskov, Jens; Huusom, Jakob Kjøbsted / **Optimal operation and stabilising control of the concentric heatintegrated distillation column (HIDiC)**. *Computers & Chemical Engineering*, Vol. 96, 2017, pp. 196-211.
- Bjørner, Martin G.; Sin, Gürkan; Kontogeorgis, Georgios M. / **Uncertainty analysis of the CPA and a quadrupolar CPA equation of state—With emphasis on  $\text{CO}_2$** . *Fluid Phase Equilibria*, Vol. 414, 2016, pp. 29-47.
- Bjørner, Martin Gamel; Kontogeorgis, Georgios / **Modelling the phase equilibria of multicomponent mixtures containing  $\text{CO}_2$ , alkanes, water, and/or alcohols using the quadrupolar CPA equation of state**. *Molecular Physics*, Vol. 114, No. 18, 2016, pp. 2641-2654.
- Boiocchi, Riccardo; Gernaey, Krist; Sin, Gürkan / **Systematic design of membership functions for fuzzy-logic control: A case study on one-stage partial nitrification/anammox treatment systems**. *Water Research*, Vol. 102, 2016, pp. 346-361.
- Bolic, Andrijana; Larsson, Hilde Kristina; Hugelier, Siewert; Eliasson Lantz, Anna; Krühne, Ulrich; Gernaey, Krist / **A flexible well-mixed milliliterscale reactor with high oxygen transfer rate for microbial cultivations**. *Chemical Engineering Journal*, Vol. 303, 2016, pp. 655-666.
- Burniol Figols, Anna; Cenian, Katarzyna; Skiadas, Ioannis V.; Gavala, Hariklia N. / **Integration of chlorogenic acid recovery and bioethanol production from spent coffee grounds**. *Biochemical Engineering Journal*, Vol. 116, 2016, pp. 54-64.
- Cai, Weiwei; Han, Tingting; Guo, Zechong; Varrone, Cristiano; Wang, Aijie; Liu, Wenzong / **Methane production enhancement by an independent cathode in integrated anaerobic reactor with microbial electrolysis**. *Bioresource Technology*, Vol. 208, 2016, pp. 13-18.
- Cao, Xiaotong; Luo, Jianquan; Woodley, John; Wan, Yinhua / **Bioinspired Multifunctional Membrane for Aquatic Micropollutants Removal**. *A C S Applied Materials and Interfaces*, Vol. 8, No. 44, 2016, pp. 30511-30522.
- Castillo, A.; Cheali, Peam; Gómez, V.; Comas, J.; Poch, M.; Sin, Gürkan / **An integrated knowledge-based and optimization tool for the sustainable selection of wastewater treatment process concepts**. *Environmental Modelling & Software*, Vol. 84, 2016, pp. 177-192.
- Cheali, Peam; Posada, John A.; Gernaey, Krist; Sin, Gürkan / **Economic risk analysis and critical comparison of optimal biorefinery concepts**. *Biofuels, Bioproducts and Biorefining*, Vol. 10, No. 4, 2016, pp. 435-445.
- Christensen, Jakob M.; Grunwaldt, Jan-Dierk; Jensen, Anker D. / **Importance of the oxygen bond strength for catalytic activity in soot oxidation**. *Applied Catalysis B: Environmental*, Vol. 188, 2016, pp. 235-244.
- Christiansen, Caspar; Stolberg-Rohr, Thomine; Fateev, Alexander; Clausen, Sønnik / **High temperature and high pressure gas cell for quantitative spectroscopic measurements**. *Journal of Quantitative Spectroscopy & Radiative Transfer*, Vol. 169, 2016, pp. 96-103.
- Collalti, A.; Marconi, S.; Ibrom, Andreas; Trotta, C.; Anav, A.; D'andrea, E.; Matteucci, G.; Montagnani, L.; Gielen, B.; Mammarella, I.; Grünwald, T.; Knohl, A.; Berninger, F.; Zhao, Yichun; Valentini, R.; Santini, M. / **Validation of 3D-CMCC Forest Ecosystem Model (v.5.1) against eddy covariance data for 10 European forest sites**. *Geoscientific Model Development*, Vol. 9, No. 2, 2016, pp. 479-504.
- Colom, Juan M.; Alzueta, María U.; Christensen, Jakob Munkholt; Glarborg, Peter; Cordtz, Rasmus Fauriskov; Schramm, Jesper / **Importance of Vanadium-Catalyzed Oxidation of  $\text{SO}_2$  to  $\text{SO}_3$  in Two-Stroke Marine Diesel Engines**. *Energy & Fuels*, Vol. 30, No. 7, 2016, pp. 6098-6102.
- Costanzo, Salvatore; Huang, Qian; Ianniruberto, Giovanni; Marrucci, Giuseppe; Hassager, Ole; Vlassopoulos, Dimitris / **Shear and Extensional Rheology of Polystyrene Melts and Solutions with the Same Number of Entanglements**. *Macromolecules*, Vol. 49, No. 10, 2016, pp. 3925-3935.
- 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*, 2016.
- Dotsenko, Gleb; Lange, Lene / **Enzyme Enhanced Protein Recovery from Green Biomass Pulp**. *Waste and Biomass Valorization*, 2016.



Dotsenko, Gleb; Nielsen, Michael Krogsgaard; Lange, Lene / **Statistical model semiquantitatively approximates arabinoxyloligosaccharides' structural diversity**. Carbohydrate Research, Vol. 426, 2016, pp. 9-14.

Dotsenko, Gleb; Osipov, D. O.; Zorov, I. N.; Sinitsyn, A. pp. / **Comparative analysis of the effect of pretreating aspen wood with aqueous and aqueous-organic solutions of sulfuric and nitric acid on its reactivity during enzymatic hydrolysis**. Catalysis in Industry, Vol. 8, No. 1, 2016, pp. 88-94.

Dotsenko, Gleb; Tong, Xiaoxue; Pilgaard, Bo; Kamp Busk, Peter; Lange, Lene / **Acidic-alkaline ferulic acid esterase from *Chaetomium thermophilum* var. *dissitum*: Molecular cloning and characterization of recombinant enzyme expressed in *Pichia pastoris***. Biocatalysis and Agricultural Biotechnology, Vol. 5, 2016, pp. 48-55.

Duhn, Jakob Dragsbæk; Jensen, Anker Degn; Wedel, Stig; Wix, Christian / **Optimization of a new flow design for solid oxide cells using computational fluid dynamics modelling**. Journal of Power Sources, Vol. 336, 2016, pp. 261-271.

Economou, Ioannis G.; Kontogeorgis, Georgios / **Thermodynamics 2015 Conference Copenhagen, Denmark, 15-18 September 2015**. Molecular Physics, Vol. 114, No. 18, 2016, pp. 2569-2573.

Ehgartner, Josef; Sulzer, Philipp; Burger, Tobias; Kasjanow, Alice; Bouwes, Dominique; Krühne, Ulrich; Klimant, Ingo; Mayr, Torsten / **Online analysis of oxygen inside silicon-glass microreactors with integrated optical sensors**. Sensors and Actuators B: Chemical, Vol. 228, 2016, pp. 748-757.

Fassheber, Nancy; Friedrichs, Gernot; Marshall, Paul; Glarborg, Peter / **Glyoxal Oxidation Mechanism: Implications for the Reactions  $\text{HCO} + \text{O}_2$  and  $\text{OCHCHO} + \text{HO}_2$** . Journal of Physical Chemistry Part A: Molecules, Spectroscopy, Kinetics, Environment and General Theory, Vol. 119, No. 28, 2015, pp. 7305-7315.

Feng, Ping; Lin, Weigang; Jensen, Peter Arendt; Song, Wenli; Hao, Lifang; Raffelt, Klaus; Dam-Johansen, Kim / **Entrained flow gasification of coal/ bio-oil slurries**. Energy, Vol. 111, 2016, pp. 793-802.

Ferrari, A.; Gutierrez, S.; Sin, Gürkan / **Modeling a production scale milk drying process: parameter estimation, uncertainty and sensitivity analysis**. Chemical Engineering Science, Vol. 152, 2016, pp. 301-310.

Flores Alsina, Xavier; Solon, Kimberly; Kazadi Mbamba, Christian; Tait, Stephan; Gernaey, Krist; Jeppsson, Ulf; Batstone, Damien J. / **Modelling phosphorus (P), sulfur (S) and iron (Fe) interactions for dynamic simulations of anaerobic digestion processes**. Water Research, Vol. 95, 2016, pp. 370-382.

Folens, Karel; Mortier, Séverine Thérèse F C; Baeten, Janis; Couvreur, Karen; Michelet, Robin; Gernaey, Krist; De Beer, Thomas; Du Laing, Gijs; Nopens, Ingmar / **Modelling and sensitivity analysis of urinary platinum excretion in anticancer chemotherapy for the recovery of platinum**. Sustainable Chemistry and Pharmacy, Vol. 4, 2016, pp. 46-56.

Fosbol, Emil L.; Fosbøl, Philip Loldrup; Rerup, Sofie; Ostergaard, Lauge; Ahmed, Mohammed H.; Butt, Jawad; Davidsen, Julie; Shanmuganathan, Nirusiya; Juul, Simon; Lewinter, Christian / **Low immediate scientific yield of the PhD among medical doctors**. BMC Medical Education, Vol. 16, No. 1, 189, 2016.

Frost, Michael Grynnerup; Kontogeorgis, Georgios; von Solms, Nicolas; Solbraa, Even / **Modelling of phase equilibrium of North Sea oils with water and MEG**. Fluid Phase Equilibria, Vol. 424, 2016, pp. 79-89.

Frutiger, Jerome; Andreassen, Jesper Graa; Liu, Wei; Spliethoff, Hartmut; Haglund, Fredrik; Abildskov, Jens; Sin, Gürkan / **Working fluid selection for organic Rankine cycles—Impact of uncertainty of fluid properties**. Energy, Vol. 109, 2016, pp. 987-997.

Frutiger, Jerome; Marcarie, Camille; Abildskov, Jens; Sin, Gürkan / **Group-Contribution based Property Estimation and Uncertainty analysis for Flammability-related Properties**. Journal of Hazardous Materials, Vol. 318, 2016, pp. 783-793.

Fung, Ka Y.; Ng, Ka M.; Zhang, Lei; Gani, Rafiqul / **A grand model for chemical product design**. Computers and Chemical Engineering, Vol. 91, 2016, pp. 15-27.

Furlan, Felipe F.; Costa, Caliane B B; Secchi, Argimiro R.; Woodley, John; Giordano, Roberto C. / **Retro-Techno-Economic Analysis: Using (Bio)Process Systems Engineering Tools to Attain Process Target Values**. Industrial & Engineering Chemistry Research, Vol. 55, No. 37, 2016, pp. 9865-9872.

Gaspar, Jozsef; Fosbøl, Philip Loldrup / **Practical enhancement factor model based on GM for multiple parallel reactions: Piperazine (PZ)  $\text{CO}_2$  capture**. Chemical Engineering Science, Vol. 158, 2017, pp. 257-266.

García-Pintos, Delfina; Voss, Johannes; Jensen, Anker Degn; Studt, Felix / **Hydrodeoxygenation of Phenol to Benzene and Cyclohexane on Rh(111) and Rh(211) Surfaces: Insights from Density Functional Theory**. The Journal of Physical Chemistry Part C: Nanomaterials, Interfaces and Hard Matter, Vol. 120, No. 33, 2016, pp. 18529-18537.

Gardini, Diego; Christensen, Jakob M.; Damsgaard, Christian Danvad; Jensen, Anker D.; Wagner, Jakob B. / **Visualizing the mobility of silver during catalytic soot oxidation**. Applied Catalysis B: Environmental, Vol. 183, 2016, pp. 28-36.

Gaspar, Jozsef; Fosbøl, Philip Loldrup / **Simulation and multivariable optimization of post-combustion capture using piperazine**. International Journal of Greenhouse Gas Control, Vol. 49, 2016, pp. 227-238.

Gaspar, Jozsef; Ricardez-Sandoval, Luis; Jørgensen, John Bagterp; Fosbøl, Philip Loldrup / **Controllability and flexibility analysis of  $\text{CO}_2$  post-combustion capture using piperazine and MEA**. International Journal of Greenhouse Gas Control, Vol. 51, 2016, pp. 276-289.

Gersen, Sander; van Essen, Martijn; Darneveil, Harry; Hashemi, Hamid; Rasmussen, Christian Tihic; Christensen, Jakob Munkholt; Glarborg, Peter; Levinsky, Howard / **Experimental and Modeling Investigation of the Effect of  $\text{H}_2\text{S}$  Addition to Methane on the Ignition and Oxidation at High Pressures**. Energy & Fuels, 2016, pp. 8.

Gladis, Arne; Bondesson, Pia-Maria; Galbe, Mats; Zacchi, Guido / **Influence of different SSF conditions on ethanol production from corn stover at high solids loadings**. Energy Science & Engineering, Vol. 3, No. 5, 2015, pp. 481-489.

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; Troe, Juergen / **Temperature and Pressure Dependence of the Reaction  $\text{S} + \text{CS} (+\text{M}) \rightarrow \text{CS}_2 (+\text{M})$** . Journal of Physical Chemistry Part A: Molecules, Spectroscopy, Kinetics, Environment and General Theory, Vol. 119, No. 28, 2015, pp. 7277-7281.

Grivel, Jean-Claude; Alexiou, Aikaterini; Namazkar, Shahla; Pitillas, Andrea / **Effect of Platinum Group Metal Doping in Magnesium Diboride Wires**. IEEE Transactions on Applied Superconductivity, Vol. 26, No. 3, 6200505, 2016.

Grivel, Jean-Claude; Pitillas, A.; Namazkar, Shahla; Alexiou, A.; Holte, Olfert Joakim / **Preparation and characterization of  $\text{MgB}_2$  with Pd, Pt and Re doping**. Physica C: Superconductivity and its Applications, Vol. 520, 2016, pp. 37-41.

Gundersen Deslauriers, Maria; Tufvesson, Pär; Rackham, Emma J.; Lloyd, Richard C.; Woodley, John / **A Rapid Selection Procedure for Simple Commercial Implementation of omega-Transaminase Reactions**. Organic Process Research and Development, Vol. 20, No. 3, 2016, pp. 602-608.

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, 2016.

Hansen, Veronika; Hauggaard-Nielsen, Henrik; Petersen, Carsten Tilbæk; Mikkelsen, Teis Nørgaard; Müller-Stöver, Dorette Sophie / **Effects of gasification biochar on plant-available water capacity and plant growth in two contrasting soil types**. Soil & Tillage Research, Vol. 161, 2016, pp. 1-9.

Hashemi, Hamid; Christensen, Jakob Munkholt; Gersen, Sander; Levinsky, Howard; Klippenstein, Stephen J.; Glarborg, Peter / **High-pressure oxidation of methane**. Combustion and Flame, Vol. 172, 2016, pp. 349-364.

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, 2016.

- Heintz, Søren; Mitic, Aleksandar; Ringborg, Rolf Hoffmeyer; Krühne, Ulrich; Woodley, John; Gernaey, Krist / **A microfluidic toolbox for the development of in-situ product removal strategies in biocatalysis**. Journal of Flow Chemistry, Vol. 6, No. 1, 2016, pp. 18-26.
- Hengeller, Ludovica; Huang, Qian; Dorokhin, Andriy; Alvarez, Nicolas J.; Almdal, Kristoffer; Hassager, Ole / **Stress relaxation of bi-disperse polystyrene melts : Exploring the interactions between long and short chains in non-linear rheology**. Rheologica Acta, Vol. 55, No. 4, 2016, pp. 303-314.
- Huang, Qian; Agostini, Serena; Hengeller, Ludovica; Shivokhin, Maksim; Alvarez, Nicolas J.; Hutchings, Lian R.; Hassager, Ole / **Dynamics of Star Polymers in Fast Extensional Flow and Stress Relaxation**. Macromolecules, Vol. 49, No. 17, 2016, pp. 6694-6699.
- Huang, Qian; Alvarez, Nicolas J.; Shabbir, Aamir; Hassager, Ole / **Multiple Cracks Propagate Simultaneously in Polymer Liquids in Tension**. Physical Review Letters, Vol. 117, No. 8, 087801, 2016.
- 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; Mangnus, Marc; Alvarez, Nicolas J.; Koopmans, Rudy; Hassager, Ole / **A new look at extensional rheology of low-density polyethylene**. Rheologica Acta, Vol. 55, No. 5, 2016, pp. 343-350.
- Huang, Qian; Rasmussen, Henrik K. / **Stress relaxation following uniaxial extension of polystyrene melt and oligomer dilutions**. Journal of Rheology, Vol. 60, No. 3, 2016, pp. 465-471.
- Huusom, Jakob Kjøbsted; Gani, Rafiqul / **Preface. Computers and Chemical Engineering**, Vol. 91, 2016, pp. 1-2.
- Hvilsted, Søren / **Conducting Polymeric Materials**. Macromolecular Chemistry and Physics, Vol. 217, No. 10, 2016, pp. 1107.
- Ingvordsen, Cathrine Heinz; Gislum, René; Jørgensen, Johannes Ravn; Mikkelsen, Teis Nørgaard; Stockmarr, Anders; Bagger Jørgensen, Rikke / **Grain protein concentration and harvestable protein under future climate conditions**. A study of 108 spring barley accessions. Journal of Experimental Botany, Vol. 67, No. 8, 2016, pp. 2151-2158.
- Jakobsen, Iver; Smith, Sally E.; Smith, F. Andrew; Watts-Williams, Stephanie J.; Clausen, Signe Sandbech; Grønlund, Mette / **Plant growth responses to elevated atmospheric CO<sub>2</sub> are increased by phosphorus sufficiency but not by arbuscular mycorrhizas**. Journal of Experimental Botany, Vol. 67, No. 21, 2016, pp. 6173-6186.
- 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, 2016.
- Johansen, Joakim M.; Jensen, Peter A.; Glarborg, Peter; Mancini, Marco; Weber, Roman; Mitchell, Reginald E. / **Extension of apparent devolatilization kinetics from thermally thin to thermally thick particles in zero dimensions for woody biomass**. Energy, Vol. 95, 2016, pp. 279-290.
- Jurado, E.; Antonopoulou, G.; Lyberatos, G.; Gavala, Hariklia N.; Skiadas, Ioannis V. / **Continuous anaerobic digestion of swine manure: ADM1-based modelling and effect of addition of swine manure fibers pretreated with aqueous ammonia soaking**. Applied Energy, Vol. 172, 2016, pp. 190-198.
- 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**. Biochemical Engineering Journal, 2016.
- Kalyani, D. C.; Munk, L.; Mikkelsen, J. D.; Meyer, A. S. / **Molecular and biochemical characterization of a new thermostable bacterial laccase from *Meiothermus ruber* DSM 1279**. R S C Advances, Vol. 6, No. 5, 2016, pp. 3910-3918.
- Kamal, Muhammad Shahzad; Hussein, Ibnelwaleed A.; Sultan, Abdullah S.; von Solms, Nicolas / **Application of various water soluble polymers in gas hydrate inhibition**. Renewable and Sustainable Energy Reviews, Vol. 60, 2016, pp. 206-225.
- Kamp, Andreas; Østergård, Hanne / **Environmental sustainability assessment of fruit cultivation and processing using fruit and cocoa residues for bioenergy and compost**. Case study from Ghana. Journal of Cleaner Production, Vol. 129, 2016, pp. 329-340.
- Kamp, Andreas; Østergård, Hanne; Bolwig, Simon / **Environmental Assessment of Integrated Food and Cooking Fuel Production for a Village in Ghana**. Sustainability, Vol. 8, No. 5, 404, 2016.
- Katika, Konstantina; Ahkami, Mehrdad; Fosbøl, Philip Loldrup; Halim, Amalia Yunita; Shapiro, Alexander; Thomsen, Kaj; Xiarchos, Ioannis; Fabricius, Ida Lykke / **Comparative analysis of experimental methods for quantification of small amounts of oil in water**. Journal of Petroleum Science and Engineering, Vol. 147, 2016, pp. 459-467.
- Kiil, Søren / **Mathematical modeling of pigment dispersion taking into account the full agglomerate particle size distribution**. Journal of Coatings Technology and Research, 2016.
- Kim, Sun Hyung; Anantpinijwatna, Amata; Kang, Jeong Won; Gani, Rafiqul / **Analysis and modeling of alkali halide aqueous solutions**. Fluid Phase Equilibria, Vol. 412, 2016, pp. 177-198.
- Kirkensgaard, Jacob J K; Hengeller, Ludovica; Dorokhin, Andriy; Huang, Qian; Garvey, Christopher J.; Almdal, Kristoffer; Hassager, Ole; Mortensen, Kell / **Nematic effects and strain coupling in entangled polymer melts under strong flow**. Physical Review E (Statistical, Nonlinear, and Soft Matter Physics), Vol. 94, No. 2, 020502, 2016.
- Kongpanna, Pichayapan; Babi, Deenesh K.; Pavarajarn, Varong; Assabumrungrat, Suttichai; Gani, Rafiqul / **Systematic methods and tools for design of sustainable chemical processes for CO<sub>2</sub> utilization**. Computers and Chemical Engineering, Vol. 87, 2016, pp. 125-144.
- Kumar, Ashish; Dhondt, Jens; Vercruysse, Jurgen; De Leersnyder, Fien; Vanhoorne, Valerie; Vervaet, Chris; Remon, Jean Paul; Gernaey, Krist; De Beer, Thomas; Nopens, Ingmar / **Development of a process map: A step towards a regime map for steady-state high shear wet twin screw granulation**. Powder Technology, Vol. 300, 2016, pp. 73-82.
- Kumar, Ashish; Vercruysse, Jurgen; Mortier, Severine T. F. C.; Vervaet, Chris; Remon, Jean Paul; Gernaey, Krist; De Beer, Thomas; Nopens, Ingmar / **Modelbased analysis of a twin-screw wet granulation system for continuous solid dosage manufacturing**. Computers and Chemical Engineering, Vol. 89, 2016, pp. 62-70.
- Kumar Tula, Anjan; Befort, Bridgette; Garg, Nipun; Camarda, Kyle V.; Gani, Rafiqul / **Sustainable process design & analysis of hybrid separations**. Computers & Chemical Engineering, 2016.
- Kvamsdal, Hanne M.; Ehlers, Sören; Kather, Alfons; Khakharia, Purvil; Nienoord, Michiel; Fosbøl, Philip Loldrup / **Optimizing integrated reference cases in the OCTAVIUS project**. International Journal of Greenhouse Gas Control, Vol. 50, 2016, pp. 23-36.
- Lange, Lene; Huang, Yuhong; Kamp Busk, Peter / **Microbial decomposition of keratin in nature – a new hypothesis of industrial relevance**. Applied Microbiology and Biotechnology, Vol. 100, No. 5, 2016, pp. 2083-2096.
- Lehmann, Linda Olkjær; Petersen, Nanna; I. Jørgensen, Christian; Olsson, Lisbeth; Stocks, Stuart M.; Jørgensen, Henrik S.; Hobley, Timothy John / **Linking Hydrolysis Performance to *Trichoderma reesei* Cellulolytic Enzyme Profile**. Biotechnology and Bioengineering, Vol. 113, No. 5, 2016, pp. 1001-1010.
- Lezyk, Mateusz Jakub; Jers, Carsten; Kjærulff, Louise; Gotfredsen, Charlotte Held; Mikkelsen, Maria D.; Mikkelsen, Jørn Dalgaard / **Novel  $\alpha$ -L-Fucosidases from a Soil Metagenome for Production of Fucosylated Human Milk Oligosaccharides**. P L o S One, Vol. 11, No. 1, e0147438, 2016.
- Liang, Xiaodong; Michelsen, Michael Locht; Kontogeorgis, Georgios / **A density gradient theory based method for surface tension calculations**. Fluid Phase Equilibria, Vol. 428, 2016, pp. 153-163.
- Liang, Xiaodong; Michelsen, Michael Locht; Kontogeorgis, Georgios / **Pitfalls of using the geometric-mean combining rule in the density gradient theory**. Fluid Phase Equilibria, Vol. 415, 2016, pp. 75-83.
- Liu, Huang; Guo, Ping; Regueira Muñiz, Teresa; Wang, Zhouhua; Du, Jianfen; Chen, Guangjin / **Irreversible Change of the Pore Structure of ZIF-8 in Carbon Dioxide**



**Capture with Water Coexistence.** Journal of Physical Chemistry C, Vol. 120, No. 24, 2016, pp. 13287-13294.

Liu, Ming; Meyer, Anne S.; Fernando, Dinesh; Silva, Diogo Alexandre Santos; Daniel, Geoffrey; Thygesen, Anders / **Effect of pectin and hemicellulose removal from hemp fibres on the mechanical properties of unidirectional hemp/epoxy composites.** Composites Part A: Applied Science and Manufacturing, Vol. 90, 2016, pp. 724-735.

Liu, Ming; Silva, Diogo Alexandre Santos; Fernando, Dinesh; Meyer, Anne S.; Madsen, Bo; Daniel, Geoffrey; Thygesen, Anders / **Controlled retting of hemp fibres: Effect of hydrothermal pre-treatment and enzymatic retting on the mechanical properties of unidirectional hemp/epoxy composites.** Composites Part A: Applied Science and Manufacturing, Vol. 88, 2016, pp. 253-262.

Liu, Shuai; He, Fang; Huang, Zhen; Zheng, Anqing; Feng, Yipeng; Shen, Yang; Li, Haibin; Wu, Hao; Glarborg, Peter / **Screening of NiFe<sub>2</sub>O<sub>4</sub> Nanoparticles as Oxygen Carrier in Chemical Looping Hydrogen Production.** Energy and Fuels, Vol. 30, No. 5, 2016, pp. 4251-4262.

Liu, Wenzong; Cai, Weiwei; Guo, Zechong; Yang, Chunxue; Varrone, Cristiano; Wang, Aijie / **Microbial electrolysis contribution to anaerobic digestion of waste activated sludge, leading to accelerated methane production.** Renewable Energy, Vol. 91, 2016, pp. 334-339.

Liu, Wenzong; He, Zhangwei; Yang, Chunxue; Zhou, Aijuan; Guo, Zechong; Liang, Bin; Varrone, Cristiano; Wang, Ai-jie / **Microbial network for waste activated sludge cascade utilization in an integrated system of microbial electrolysis and anaerobic fermentation.** Biotechnology for Biofuels, Vol. 9, No. 83, 2016.

Liu, Xinyan; Huang, Ying; Zhao, Yongsheng; Gani, Rafiqul; Zhang, Xiangping; Zhang, Suojiao / **Ionic Liquid Design and Process Simulation for Decarbonization of Shale Gas.** Industrial and Engineering Chemistry Research, Vol. 55, No. 20, 2016, pp. 5931-5944.

Liu, Yanrong; Thomsen, Kaj; Nie, Yi; Zhang, Suo-Jiang; Meyer, Anne S. / **Predictive screening of ionic liquids for dissolving cellulose and experimental verification.** Green Chemistry, Vol. 18, No. 23, 2016, pp. 6246-6254.

Liu, Yilan; Yang, Maohua; Yan, Daojiang; Cheng, Wanwan; Thygesen, Anders; Chen, Ruonan; Xing, Jianmin; Wang, Qinhong; Ma, Yanhe; Isalan, Mark (Editor) / **PCR-Based Seamless Genome Editing with High Efficiency and Fidelity in Escherichia coli.** PLoS One, Vol. 11, No. 3, 2016, pp. e0149762.

Lopez, Jorge Gimenez; Rasmussen, Christian Tihic; Hashemi, Hamid; Alzueta, Maria; Gao, Yide; Marshall, Paul; Goldsmith, C. Franklin; Glarborg, Peter / **Experimental and Kinetic Modeling Study of C<sub>2</sub>H<sub>2</sub> Oxidation at High Pressure.** International Journal of Chemical Kinetics, Vol. 48, No. 11, 2016, pp. 724-738.

Loureiro da Costa Lira Gargalo, Carina; Cheali, Peam; Posada, John A.; Carvalho, Ana; Gernaey, Krist; Sin, Gürkan / **Assessing the environmental sustainability of early stage design for bioprocesses under uncertainties: An analysis of glycerol bioconversion.** Journal of Cleaner Production, Vol. 139, 2016, pp. 1245-1260.

Loureiro da Costa Lira Gargalo, Carina; Cheali, Peam; Posada, John A.; Gernaey, Krist; Sin, Gürkan / **Economic Risk Assessment of Early Stage Designs for Glycerol 2 Valorization in Biorefinery Concepts.** Industrial & Engineering Chemistry Research, Vol. 55, No. 24, 2016, pp. 6801-6814.

Loureiro da Costa Lira Gargalo, Carina; Sin, Gürkan; Carvalho, Ana; Gernaey, Krist; Sin, Gürkan / **A framework for techno-economic & environmental sustainability analysis by risk assessment for conceptual process evaluation.** Biochemical Engineering Journal, Vol. 116, 2016, pp. 146-156.

Lu, Zhimin; Jian, Jie; Jensen, Peter Arendt; Wu, Hao; Glarborg, Peter / **Influence of Torrefaction on Single Particle Combustion of Wood.** Energy and Fuels, Vol. 30, No. 7, 2016, pp. 5772-5778.

Lythcke-Jørgensen, Christoffer Ernst; Clausen, Lasse Røngaard; Algren, Loui; Bavnghøj Hansen, Anders; Münster, Marie; Gadsbøll, Rasmus Østergaard; Haglind, Fredrik / **Optimization of a flexible multigeneration system based on wood chip gasification and methanol production.** Applied Energy, 2016.

M. Weiss, Florian; Madsen, Frederikke Bahrt; Töpfer, Tino; Osman, Bekim; Leung, Vanessa; Müller, Bert / **Molecular beam deposition of high-permittivity polydimethylsiloxane for nanometer-thin elastomer films in dielectric actuators.** Materials & Design, Vol. 105, 2016, pp. 106-113.

Ma, Teng; Fan, Chuigang; Hao, Lifang; Li, Songgeng; Song, Wenli; Lin, Weigang / **Biomass-Ash-Induced Agglomeration in a Fluidized Bed. Part 1: Experimental Study on the Effects of a Gas Atmosphere.** Energy & Fuels, Vol. 30, No. 8, 2016, pp. 6395-6404.

Ma, Teng; Fan, Chuigang; Hao, Lifang; Li, Songgeng; Song, Wenli; Lin, Weigang / **Fusion characterization of biomass ash.** Thermochimica Acta, Vol. 638, 2016, pp. 1-9.

Madsen, Frederikke Bahrt; Dagaard, Anders Egede; Hvilsted, Søren; Skov, Anne Ladegaard / **The Current State of Silicone-Based Dielectric Elastomer Transducers.** Macromolecular Rapid Communications, Vol. 37, No. 5, 2016, pp. 378-413.

Madsen, Frederikke Bahrt; Yu, Liyun; Mazurek, Piotr Stanislaw; Skov, Anne Ladegaard / **A simple method for reducing inevitable dielectric loss in highpermittivity dielectric elastomers.** Smart Materials and Structures, Vol. 25, No. 7, 075018, 2016.

Madsen, Frederikke Bahrt; Yu, Liyun; Skov, Anne Ladegaard / **Self-Healing, High-Permittivity Silicone Dielectric Elastomer.** ACS Macro Letters, Vol. 5, 2016, pp. 1196-1200.

Madsen, Frederikke Bahrt; Zakaria, Shamsul Bin; Yu, Liyun; Skov, Anne Ladegaard / **Mechanical and Electrical Ageing Effects on the Long-Term Stretching of Silicone Dielectric Elastomers with Soft Fillers : Long-Term Stretching of Silicone Dielectric Elastomers.** Advanced Engineering Materials, 2016.

Manns, Dirk Martin; Nyffenegger, Christian; Saake, B.; Meyer, Anne S. / **Impact of different alginate lyases on combined cellulase-lyase saccharification of brown seaweed.** RSC Advances, Vol. 6, No. 51, 2016, pp. 45392-45401.

Mansouri, Seyed Soheil; Sales-Cruz, Mauricio; Huusom, Jakob Kjøbsted; Gani, Rafiqul / **Systematic Integrated Process Design and Control of Binary Element Reactive Distillation Processes.** AIChE Journal, Vol. 62, No. 9, 2016, pp. 3137-3154.

Mansouri, Seyed Soheil; Sales-Cruz, Mauricio; Huusom, Jakob Kjøbsted; Gani, Rafiqul / **Systematic Integrated Process Design and Control of Reactive Distillation Processes Involving Multi-elements.** Chemical Engineering Research & Design, Vol. 115, No. Part B, 2016, pp. 348-364.

Marizza, Paolo; Abrami, M.; Keller, Stephan Sylvest; Posocco, P.; Laurini, E.; Goswami, Kaustav; Skov, Anne Ladegaard; Boisen, Anja; Larobina, D.; Grassi, G.; Grassi, M. / **Synthesis and characterization of UV photocrosslinkable hydrogels with poly(N-vinyl-2-pyrrolidone): Determination of the network mesh size distribution.** International Journal of Polymeric Materials and Polymeric Biomaterials, Vol. 65, No. 10, 2016, pp. 516-525.

Mazurek, P.; Hvilsted, S.; Skov, A. L. / **Green silicone elastomer obtained from a counterintuitively stable mixture of glycerol and PDMS.** Polymer, Vol. 87, 2016, pp. 1-7.

Mazurek, Piotr Stanislaw; Yu, Liyun; Gerhard, R.; Wirges, W.; Skov, Anne Ladegaard / **Glycerol as highpermittivity liquid filler in dielectric silicone elastomers.** Journal of Applied Polymer Science, Vol. 133, No. 43, 44153, 2016.

Mbamba, Christian Kazadi; Flores Alsina, Xavier; Batstone, Damien John; Tait, Stephan / **Validation of a plant-wide phosphorus modelling approach with minerals precipitation in a full-scale WWTP.** Water Research, Vol. 100, 2016, pp. 169-183.

Mears, Lisa; Nørregaard, Rasmus; Sin, Gürkan; Gernaey, Krist V.; Stocks, Stuart M.; Albæk, Mads O.; Villez, Kris / **Functional Unfold Principal Component Regression Methodology for Analysis of Industrial Batch Process Data.** AIChE Journal, Vol. 62, No. 6, 2016, pp. 1986-1994.

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, 2016.

Meier, Robert J.; Gundersen Deslauriers, Maria; Woodley, John; Schürmann, Martin / **A Practical and Fast Method To Predict the Thermodynamic Preference of om-ga-Transaminase-Based Transformations.** ChemCatChem, Vol. 7, No. 17, 2015, pp. 2594-2597.

Mekasha, Sophanit; Toupalová, Hana; Linggadjaja, Eka; Tolani, Harish A.; Anděra, Ladislav; Arntzen, Magnus; Vaaje-Kolstad, Gustav; Eijssink, Vincent G H; Witttrup Agger, Jane / **A novel analytical method for Dglucosamine quantification and its application in the analysis of chitosan degradation by a minimal enzyme cocktail.** Carbohydrate Research, Vol. 433, 2016, pp. 18-24.

- 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, 2016.
- Meriçer, Çağlar; Minelli, Matteo; Angelis, Maria G De; Giacinti Baschetti, Marco; Stancampiano, Augusto; Laurita, Romolo; Gherardi, Matteo; Colombo, Vittorio; Trifol Guzman, Jon; Szabo, Peter; Lindström, Tom / **Atmospheric plasma assisted PLA/microfibrillated cellulose (MFC) multilayer biocomposite for sustainable barrier application**. Industrial Crops and Products, Vol. 93, 2016, pp. 235-243.
- Mitic, Aleksandar; Skovby, Tommy; Dam-Johansen, Kim; Gernaey, Krist / **Acceleration of Anti-Markovnikov Hydroamination in the Synthesis of an Active Pharmaceutical Ingredient**. Chemical Engineering and Technology, Vol. 39, No. 10, 2016, pp. 1821-1827.
- Mohanty, Soumyaranjan; Alm, Martin; Hemmingsen, Mette; Dolatshahi-Pirouz, Alireza; Trifol Guzman, Jon; Thomsen, Peter; Dufva, Martin; Wolff, Anders; Emnéus, Jenny / **3D Printed Silicone-Hydrogel Scaffold with Enhanced Physicochemical Properties**. Biomacromolecules, Vol. 17, No. 4, 2016, pp. 1321-1329.
- Mohanty, Soumyaranjan; Kuldeep, Kuldeep; Heiskanen, Arto; Trifol Guzman, Jon; Szabo, Peter; Dufva, Martin; Emnéus, Jenny; Wolff, Anders / **Fabrication of scalable tissue engineering scaffolds with dual-pore microarchitecture by combining 3D printing and particle leaching**. Materials Science and Engineering C: Materials for Biological Applications, Vol. 61, 2016, pp. 180-189.
- Mollerup, Ane Loft; Mikkelsen, Peter Steen; Sin, Gürkan / **A methodological approach to the design of optimising control strategies for sewer systems**. Environmental Modelling & Software, Vol. 83, 2016, pp. 103-115.
- 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, 2016.
- 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, 2016.
- Morandi, Fabiana; Perrin, A.; Østergård, Hanne / **Miscanthus as energy crop: Environmental assessment of a miscanthus biomass production case study in France**. Journal of Cleaner Production, Vol. 137, 2016, pp. 313-321.
- Mortensen, Peter Mølgård; Gardini, Diego; Damsgaard, Christian Danvad; Grunwaldt, Jan-Dierk; Jensen, Peter Arendt; Wagner, Jakob Birkedal; Jensen, Anker Degn / **Deactivation of Ni-MoS<sub>2</sub> by bio-oil impurities during hydrodeoxygenation of phenol and octanol**. Applied Catalysis A: General, Vol. 523, 2016, pp. 159-170.
- 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.
- 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.
- Mortier, Séverine Thérèse F C; Van Bockstal, Pieter Jan; Nopens, Ingmar; De Beer, Thomas; Gernaey, Krist / **A Dynamic Design Space for Primary Drying During Batch Freeze-Drying**. Chimica Oggi, Vol. 34, No. 3, 2016, pp. 59-61.
- Mortier, Severine Therese F. C.; Van Bockstal, Pieter-Jan; Corver, Jos; Nopens, Ingmar; Gernaey, Krist; De Beer, Thomas / **Uncertainty analysis as essential step in the establishment of the dynamic Design Space of primary drying during freeze-drying**. European Journal of Pharmaceutics and Biopharmaceutics, Vol. 103, 2016, pp. 71-83.
- Mu, Liang; von Solms, Nicolas / **Methane Production and Carbon Capture by Hydrate Swapping**. Energy & Fuels, 2016.
- Muller-Stover, Dorette Sophie; Sun, Guotao; Kroff, Pablo; Thomsen, Sune Tjalfé; Hauggaard-Nielsen, Henrik / **Anaerobic co-digestion of perennials: Methane potential and digestate nitrogen fertilizer value: Methane potential and digestate nitrogen fertilizer value**. Journal of Plant Nutrition and Soil Science, Vol. 179, No. 6, 2016, pp. 696-704.
- Mussati, Sergio F.; Gernaey, Krist; Morosuk, Tatiana; Mussati, Miguel C. / **NLP modeling for the optimization of LiBr-H<sub>2</sub>O absorption refrigeration systems with exergy loss rate, heat transfer area, and cost as single objective functions**. Energy Conversion and Management, Vol. 127, 2016, pp. 526-544.
- 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, 2016.
- Nakhaei, Mohammadhadi; Lessani, B. / **Effects of solid inertial particles on the velocity and temperature statistics of wall bounded turbulent flow**. International Journal of Heat and Mass Transfer, 2016.
- Namavkar, Shahla; Stockmarr, Anders; Frenck, Georg; Egsgaard, Helge; Terkelsen, Thilde; Mikkelsen, Teis Nørgaard; Ingvordsen, Cathrine Heinz; Bagger Jørgensen, Rikke / **Concurrent elevation of CO<sub>2</sub>, O<sub>2</sub> and temperature severely affects oil quality and quantity in rapeseed**. Journal of Experimental Botany, Vol. 67, No. 14, 2016, pp. 4117-4125.
- Narayan, Vikas; Jensen, Peter Arendt; Henriksen, Ulrik Birk; Egsgaard, Helge; Nielsen, Rasmus Glar; Glarborg, Peter / **Behavior of Alkali Metals and Ash in a Low-Temperature Circulating Fluidized Bed (LTCFB) Gasifier**. Energy and Fuels, Vol. 30, 2016, pp. 1050-1061.
- Narayan, Vikas; Jensen, Peter Arendt; Henriksen, Ulrik Birk; Glarborg, Peter; Lin, Weigang; Nielsen, Rasmus Glar / **Defluidization in fluidized bed gasifiers using high-alkali content fuels**. Biomass & Bioenergy, Vol. 91, 2016, pp. 160-174.
- Neuefeind, J.; Skov, Anne Ladegaard; Daniels, J. E.; Honkimäki, V.; Jakobsen, B.; Oddershede, Jette; Poulsen, Henning Friis / **A multiple length scale description of the mechanism of elastomer stretching**. RSC Advances, Vol. 6, No. 98, 2016, pp. 95910-95919.
- Nguyen, Hiep Dinh; Löf, David; Hvilsted, Søren; Dagaard, Anders Egede / **Highly Branched Bio-Based Unsaturated Polyesters by Enzymatic Polymerization**. Polymer, 2016.
- Nielsen, Anne Veller Friis; Meyer, Anne S. / **Phytases for improved iron absorption**. Agro Food Industry Hi-Tech, Vol. 27, No. 1, 2016, pp. 48-51.
- Nielsen, Mette Møller; Manns, Dirk Martin; D'Este, Martina; Krause-Jensen, Dorte; Rasmussen, Michael Bo; Larsen, Martin Mørk; Alvarado-Morales, Merlin; Angelidaki, Irini; Bruhn, Annette / **Variation in biochemical composition of Saccharina latissima and Laminaria digitata along an estuarine salinity gradient in inner Danish waters**. Algal Research, Vol. 13, 2016, pp. 235-245.
- Niero, Monia; Olsen, Stig Irving / **Circular economy: To be or not to be in a closed product loop? A Life Cycle Assessment of aluminium cans with inclusion of alloying elements**. Resources, Conservation and Recycling, Vol. 114, 2016, pp. 18-31.
- Nikolic, Miroslav; Nguyen, Hiep Dinh; Dagaard, Anders Egede; Löf, David; Mortensen, Kell; Barsberg, Søren; Sanadi, Anand Ramesh / **Influence of surface modified nano silica on alkyd binder before and after accelerated weathering**. Polymer Degradation and Stability, Vol. 126, 2016, pp. 134-143.
- Nordvang, Rune Thorbjørn; Nyffenegger, Christian; Holck, Jesper; Jers, Carsten; Zeuner, Birgitte; Sundekilde, Ulrik K.; Meyer, Anne S.; Mikkelsen, Jørn Dalgaard / **It All Starts with a Sandwich: Identification of Sialidases with Trans-Glycosylation Activity**. PLoS One, Vol. 11, No. 7, 2016, pp. e0158434.
- Nørgaard, Kristian Petersen; Dam-Johansen, Kim; Català, Pere; Kiil, Søren / **Engineering model for intumescent coating behavior in a pilot-scale gasfired furnace**. AIChE Journal, Vol. 62, No. 11, 2016, pp. 3947-3962.
- Offei, Felix; Thygesen, Anders; Mensah, Moses; Tabbicca, Kwame; Fernando, Dinesh; Petrushina, Irina; Daniel, Geoffrey / **A viable electrode material for use in microbial fuel cells for tropical regions**. Energies, Vol. 9, No. 1, 35, 2016.
- 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, 2016.



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, 2016.

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<sub>2</sub> containing atmospheres.** Materials and Corrosion, 2016.

Okoro, Sunday Chukwudi; Kvisgaard, M.; Montgomery, Melanie; Jappe Frandsen, Flemming; Pantleon, Karen / **Pre-oxidation and its effect on reducing hightemperature corrosion of superheater tubes during biomass firing.** Surface Engineering, Vol. 133, 44153, 2016.

Olsen, Brian Kjærgaard; Kügler, Frauke; Jensen, Anker Degn / **Poisoning of vanadia based SCR catalysts by potassium: influence of catalyst composition and potassium mobility.** Catalysis Science & Technology, Vol. 6, 2016, pp. 2249-2260.

Palacio, Cyntia M.; Crismaru, Ciprian G.; Bartsch, Sebastian; Navickas, Vaidotas; Ditrach, Klaus; Breuer, Michael; Abu, Rohana; Woodley, John; Baldenius, Kai; Wu, Bian; Janssen, Dick B. / **Enzymatic network for production of ether amines from alcohols.** Biotechnology and Bioengineering, Vol. 113, No. 9, 2016, pp. 1853-1861.

Papadakis, Emmanouil; Kumar Tula, Anjan; Gani, Rafiqul / **Solvent selection methodology for pharmaceutical processes: Solvent swap.** Chemical Engineering Research & Design, Vol. 115, 2016, pp. 443-461.

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, 2016.

Pedersen, Michael Jørch; Skovby, Tommy; Mealy, Michael J.; Dam-Johansen, Kim; Kiil, Søren / **A Solvent-Free Base Liberation of a Tertiary Aminoalkyl Halide by Flow Chemistry.** Organic Process Research & Development, Vol. 20, No. 12, 2016, pp. 2043-2049.

Pedersen, Morten Nedergaard; Jensen, Peter Arendt; Hjuler, Klaus; Nielsen, Mads; Dam-Johansen, Kim / **Agglomeration and Deposition Behaviour of Solid Recovered Fuel.** Energy & Fuels, Vol. 30, No. 10, 2016, pp. 7858-7866.

Perozzello, Gerardo; Candeloro, Patrizio; De Grazia, Antonio; Esposito, Francesco; Allione, Marco; Coluccio, Maria Laura; Tallero, Rossana; Valpapuram, Immanuel; Tirinato, Luca; Das, Gobind; Giugni, Andrea; Torre, Bruno; Veltri, Pierangelo; Krühne, Ulrich; Della Valle, Giuseppe; Di Fabrizio, Enzo / **Microfluidic device for continuous single cells analysis via Raman spectroscopy enhanced by integrated plasmonic nanodimers.** Optics Express, Vol. 24, No. 2, 2016, pp. A180-A190.

Petersen, C. T.; Hansen, E.; Larsen, H. H.; Hansen, L. V.; Ahrenfeldt, Jesper; Hauggaard-Nielsen, H. / **Pore-size distribution and compressibility of coarse sandy subsoil with added biochar.** European Journal of Soil Science, Vol. 67, No. 6, 2016, pp. 726-736.

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, 2016.

Pierce, Brian; Wichmann, Jesper; Tran, Tam H.; Cheetamun, Roshan; Bacic, Antony; Meyer, Anne S. / **Formation of water-soluble soybean polysaccharides from spent flakes by hydrogen peroxide treatment.** Carbohydrate Polymers, Vol. 144, 2016, pp. 504-513.

Price, Jason; Nordblad, Mathias; Martel, Hannah H.; Chrabas, Brent; Wang, Huali; Nielsen, Per Munk; Woodley, John M. / **Scale-up of industrial biodiesel production to 40 m<sup>3</sup> using a liquid lipase formulation.** Biotechnology and Bioengineering, Vol. 113, No. 8, 2016, pp. 1719-1728.

Puig Arnavat, Maria; Shang, Lei; Sárossy, Zsuzsa; Ahrenfeldt, Jesper; Henriksen, Ulrik B. / **From a single pellet press to a bench scale pellet mill—Pelletizing six different biomass feedstocks.** Fuel Processing Technology, Vol. 142, 2016, pp. 27-33.

Ramesh, Hemalata; Zajkoska, Petra; Rebros, Martin; Woodley, John M. / **The effect of cultivation media and washing whole-cell biocatalysts on monoamine oxidase catalyzed oxidative desymmetrization of 3- azabicyclo[3,3,0]octane.** Enzyme and Microbial Technology, Vol. 83, 2016, pp. 7-13.

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, 2016.

Rasmussen, Helena; Mogensen, Kit H.; Jeppesen, Martin D.; Sørensen, Hanne R.; Meyer, Anne S. / **4- Hydroxybenzoic acid from hydrothermal pretreatment of oil palm empty fruit bunches—its origin and influence on biomass conversion.** Biomass & Bioenergy, Vol. 93, 2016, pp. 209-216.

Rasmussen, Henrik Koblit; Huang, Qian / **Constant interchain pressure effect in extensional flows of oligomer diluted polystyrene and poly(methyl methacrylate) melts.** Rheologica Acta, 2016.

Razmkhah, Somayeh; Mohammadifar, Mohammad Amin; Razavi, Seyed Mohammad Ali; Ale, Marcel Tutor / **Purification of cress seed (Lepidium sativum) gum: Physicochemical characterization and functional properties.** Carbohydrate Polymers, Vol. 141, 2016, pp. 166-174.

Razmkhah, Somayeh; Razavi, Seyed Mohammad Ali; Mohammadifar, Mohammad Amin; Ale, Marcel Tutor; Ahmadi Gavlighi, Hassan / **Protein-free cress seed (Lepidium sativum) gum: Physicochemical characterization and rheological properties.** Carbohydrate Polymers, Vol. 153, 2016, pp. 14-24.

Razmkhah, Somayeh; Razavi, Seyed Mohammad Ali; Mohammadifar, Mohammad Amin; Koocheki, Arash; Ale, Marcel Tutor / **Stepwise extraction of Lepidium sativum seed gum: Physicochemical characterization and functional properties.** International Journal of Biological Macromolecules, Vol. 88, 2016, pp. 553- 564.

Regueira Muñiz, Teresa; Pantelide, Georgia; Yan, Wei; Stenby, Erling Halfdan / **Density and phase equilibrium of the binary system methane + ndecane under high temperatures and pressures.** Fluid Phase Equilibria, Vol. 428, 2016, pp. 48-61.

Rehn, Gustav; Pedersen, Asbjørn Toftgaard; Woodley, John / **Application of NAD(P)H oxidase for cofactor regeneration in dehydrogenase catalyzed oxidations.** Journal of Molecular Catalysis B: Enzymatic, 2016.

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

Roh, Kosan; Frauzem, Rebecca; Gani, Rafiqul; Lee, Jay H. / **Process systems engineering issues and applications towards reducing carbon dioxide emissions through conversion technologies.** Chemical Engineering Research & Design, Vol. 116, 2016, pp. 27-47.

Roh, Kosan; Frauzem, Rebecca; Nguyen, Tuan B. H.; Gani, Rafiqul; Lee, Jay H. / **A methodology for the sustainable design and implementation strategy of CO<sub>2</sub> utilization processes.** Computers & Chemical Engineering, Vol. 91, 2016, pp. 407-421.

Roh, Kosan; Lee, Jay H.; Gani, Rafiqul / **A methodological framework for the development of feasible CO<sub>2</sub> conversion processes.** International Journal of Greenhouse Gas Control, Vol. 47, 2016, pp. 250-265.

Saagi, Ramesh; Flores Alsina, Xavier; Fu, Guangtao; Butler, David; Gernaey, Krist V.; Jeppsson, Ulf / **Catchment & sewer network simulation model to benchmark control strategies within urban wastewater systems.** Environmental Modelling & Software, Vol. 78, 2016, pp. 16-30.

Sandoval Lemus, Diego Rolando; Yan, Wei; Michelsen, Michael Loch; Stenby, Erling Halfdan / **The Phase Envelope of Multicomponent Mixtures in the Presence of a Capillary Pressure Difference.** Industrial and Engineering Chemistry Research, Vol. 55, No. 22, 2016, pp. 6530-6538.

Santa Cruz, Judith A.; Mussati, Sergio F.; Scenna, Nicolás J.; Gernaey, Krist; Mussati, Miguel C. / **Reaction invariant-based reduction of the activated sludge model ASM1 for batch applications.** Journal of Environmental Chemical Engineering, Vol. 4, No. 3, 2016, pp. 3654-3664.

Santos-Moriano, Paloma; Woodley, John; Plou, Francisco J. / **Continuous production of chitooligosaccharides by an immobilized enzyme in a dual-reactor system.** Journal of Molecular Catalysis B: Enzymatic, Vol. 133, 2016, pp. 211-217.

- Shabbir, Aamir; Huang, Qian; Chen, Quan; Colby, Ralph H.; Alvarez, Nicolas J.; Hassager, Ole / **Brittle fracture in associative polymers: the case of ionomer melts**. *Soft Matter*, Vol. 12, No. 36, 2016, pp. 7606-7612.
- Shabbir, Aamir; Javakhishvili, Irakli; Cervený, Silvana; Hvilsted, Søren; Skov, Anne Ladegaard; Hassager, Ole; Alvarez, Nicolas J. / **Linear Viscoelastic and Dielectric Relaxation Response of Unentangled UPy-Based Supramolecular Networks**. *Macromolecules*, Vol. 49, No. 10, 2016, pp. 3899-3910.
- Shahid, T.; Huang, Qian; Oosterlinck, F.; Clasen, C.; van Ruymbeke, E. / **Dynamic dilution exponent in monodisperse entangled polymer solutions**. *Soft Matter*, 2016.
- Shapiro, Alexander A. / **Mechanics of the Separating Surface for a Two-Phase Co-current Flow in a Porous Medium**. *Transport in Porous Media*, Vol. 112, No. 2, 2016, pp. 489-517.
- Sitarz, Anna K.; Mikkelsen, Jørn D.; Meyer, Anne S. / **Structure, functionality and tuning up of laccases for lignocellulose and other industrial applications**. *Critical Reviews in Biotechnology*, Vol. 36, No. 1, 2016, pp. 70-86.
- Sizikov, Valery S.; Evseev, Vadim; Fateev, Alexander; Clausen, Sønnik / **Direct and inverse problems of infrared tomography**. *Applied Optics*, Vol. 55, No. 1, 2016, pp. 208-220.
- Snip, Laura; Flores Alsina, Xavier; Aymerich, I.; Rodríguez-Mozaz, S.; Barceló, D.; Plósz, Benedek G.; Corominas, L. I.; Rodríguez-Roda, I.; Jeppsson, U.; Gernaey, Krist / **Generation of synthetic influent data to perform (micro)pollutant wastewater treatment modelling studies**. *Science of the Total Environment*, Vol. 569-570, 2016, pp. 278-290.
- Song, Yu; Hashemi, Hamid; Christensen, Jakob Munkholt; Zou, Chun; Marshall, Paul; Glarborg, Peter / **Ammonia oxidation at high pressure and intermediate temperatures**. *Fuel*, Vol. 181, 2016, pp. 358-365.
- Song, Yu; Hashemi, Hamid; Christensen, Jakob Munkholt; Zou, Chun; Haynes, Brian S.; Marshall, Paul; Glarborg, Peter / **An Exploratory Flow Reactor Study of H<sub>2</sub>S Oxidation at 30-100 Bar**. *International Journal of Chemical Kinetics*, 2016.
- Sun, Guotao; Rodrigues, Diogo De Sacadura; Thygesen, Anders; Daniel, Geoffrey; Fernando, Dinesh; Meyer, Anne S. / **Inocula selection in microbial fuel cells based on anodic biofilm abundance of *Geobacter sulfurreducens***. *Chinese Journal of Chemical Engineering*, Vol. 24, No. 3, 2016, pp. 379-387.
- Sun, Guotao; Thygesen, Anders; Meyer, Anne S. / **Cathode Assessment for Maximizing Current Generation in Microbial Fuel Cells Utilizing Bioethanol Effluent as Substrate**. *Energies*, Vol. 9, No. 5, 2016.
- Thomsen, Sune T.; Londono, Jorge E. G.; Ambye-Jensen, Morten; Heiske, Stefan; Kádár, Zsófia; Meyer, Anne S. / **Combination of ensiling and fungal delignification as effective wheat straw pretreatment**. *Biotechnology for Biofuels*, Vol. 9, No. 16, 2016.
- Toftegård, Bjarne; Clausen, Charlotte H.; Jørgensen, Sten B.; Abildskov, Jens / **New Realization of Periodic Cycled Separation**. *Industrial and Engineering Chemistry Research*, Vol. 55, No. 6, 2016, pp. 1720-1730.
- Trifol Guzman, Jon; Plackett, David; Sillard, Cecile; Szabo, Peter; Bras, Julien; Daugaard, Anders Egede / **Hybrid poly(lactic acid)/nanocellulose/nanoclay composites with synergistically enhanced barrier properties and improved thermomechanical resistance**. *Polymer International*, Vol. 65, No. 8, 2016, pp. 988-995.
- 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*, 2016.
- Trubetskaya, Anna; Jensen, Peter Arendt; Jensen, Anker Degn; Garcia Llamas, Angel David; Umeki, Kentaro; Glarborg, Peter / **Effect of fast pyrolysis conditions on biomass solid residues at high temperatures**. *Fuel Processing Technology*, Vol. 143, 2016, pp. 118-129.
- Trubetskaya, Anna; Jensen, Peter Arendt; Jensen, Anker Degn; Glarborg, Peter; Hofmann Larsen, Flemming; Andersen, Mogens Larsen / **Characterization of free radicals by electron spin resonance spectroscopy in biochars from pyrolysis at high heating rates and at high temperatures**. *Biomass & Bioenergy*, Vol. 94, 2016, pp. 117-129.
- Trubetskaya, Anna; Jensen, Peter Arendt; Jensen, Anker Degn; Llamas, Angel David Garcia; Umeki, Kentaro; Gardini, Diego; Kling, Jens; Bates, Richard; Glarborg, Peter / **Effects of several types of biomass fuels on the yield, nanostructure and reactivity of soot from fast pyrolysis at high temperatures**. *Applied Energy*, Vol. 171, 2016, pp. 468-482.
- Trubetskaya, Anna; Jensen, Peter Arendt; Jensen, Anker Degn; Steibel, Markus; Spliethoff, Hartmut; Glarborg, Peter; Larsen, Flemming Hofmann / **Comparison of high temperature chars of wheat straw and rice husk with respect to chemistry, morphology and reactivity**. *Biomass and Bioenergy*, Vol. 86, 2016, pp. 76-87.
- Tsivintzelis, Ioannis; Ali, Shahid; Kontogeorgis, Georgios / **Modeling systems relevant to the biodiesel production using the CPA equation of state**. *Fluid Phase Equilibria*, Vol. 430, 2016, pp. 75-92.
- Tzirakis, Fragkiskos; Karakatsani, Eirini; Kontogeorgis, Georgios / **Evaluation of the Cubic-Plus-Association Equation of State for Ternary, Quaternary, and Multicomponent Systems in the Presence of Monoethylene Glycol**. *Industrial & Engineering Chemistry Research*, Vol. 55, No. 43, 2016, pp. 11371-11382.
- Tzirakis, Fragkiskos; Stringari, Paolo; Coquelet, Christophe; von Solms, Nicolas; Kontogeorgis, Georgios / **Hydrate Equilibrium Data for CO<sub>2</sub>+N<sub>2</sub> System in the Presence of Tetra-n-butylammonium Fluoride (TBAF) and Mixture of TBAF and Cyclopentane (CP)**. *Journal of Chemical and Engineering Data*, Vol. 61, No. 2, 2016, pp. 1007-1011.
- Underwood, Daniel S.; Tennyson, Jonathan; Yurchenko, Sergei N.; Huang, Xinchuan; Schwenke, David W.; Lee, Timothy J.; Clausen, Sønnik; Fateev, Alexander / **ExoMol molecular line lists—XIV. The rotation-vibration spectrum of hot SO<sub>2</sub>**. *Monthly Notices of the Royal Astronomical Society*, Vol. 459, No. 4, 2016, pp. 3890-3899.
- Underwood, Daniel S.; Yurchenko, Sergei N.; Tennyson, Jonathan; Al-Refaie, Ahmed F.; Clausen, Sønnik; Fateev, Alexander / **ExoMol molecular line lists—XVII. The rotation-vibration spectrum of hot SO<sub>3</sub>**. *Monthly Notices of the Royal Astronomical Society*, Vol. 462, No. 4, 2016, pp. 162-75.
- Valverde Perez, Borja; Fuentes-Martínez, José Manuel; Flores Alsina, Xavier; Gernaey, Krist; Huusom, Jakob Kjøbsted; Plósz, Benedek G. / **Control structure design for resource recovery using the enhanced biological phosphorus removal and recovery (EBP2R) activated sludge process**. *Chemical Engineering Journal*, Vol. 296, 2016, pp. 447-457.
- Valverde Perez, Borja; Maurício Iglesias, Miguel; Sin, Gürkan / **Systematic design of an optimal control system for the SHARON-Anammox process**. *Journal of Process Control*, Vol. 39, 2016, pp. 1-10.
- Van Daele, Timothy; Fernandes del Pozo, David; Van Hauwermeiren, Daan; Gernaey, Krist; Wohlgemuth, Roland; Nopens, Ingmar / **A generic model-based methodology for quantification of mass transfer limitations in microreactors**. *Chemical Engineering Journal*, Vol. 300, 2016, pp. 193-208.
- 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.
- Vestergaard, Mette; Reinsch, Sabine; Bengtson, Per; Ambus, Per; Christensen, Søren / **Enhanced priming of old, not new soil carbon at elevated atmospheric CO<sub>2</sub>**. *Soil Biology & Biochemistry*, Vol. 100, 2016, pp. 140-148.
- von Freiesleben, Pernille; Spødsberg, Nikolaj; Holberg Blicher, Thomas; Anderson, Lars; Jørgensen, Henning; Stålbrand, Henrik; Meyer, Anne S.; Krogh, Kristian B. R. M. / **An *Aspergillus nidulans* GH26 endo-β-mannanase with a novel degradation pattern on highly substituted galactomannans**. *Enzyme and Microbial Technology*, Vol. 83, 2016, pp. 68-77.
- Waseem Arshad, Muhammad; von Solms, Nicolas; Thomsen, Kaj / **Thermodynamic modeling of liquid-liquid phase change solvents for CO<sub>2</sub> capture**. *International Journal of Greenhouse Gas Control*, Vol. 53, 2016, pp. 401-424.



- Wilkens, Casper; Andersen, Susan; Petersen, Bent O.; Li, An; Busse-Wicher, Marta; Birch, Johnny; Cockburn, Darrell; Nakai, Hiroyuki; Christensen, Hans Erik Mølager; Kragelund, Birthe B.; Dupree, Paul; McCleary, Barry; Hinds Gaul, Ole; Abou Hachem, Maher; Svensson, Birte / **An efficient arabinoxylandebanching  $\alpha$ -l-arabinofuranosidase of family GH62 from *Aspergillus nidulans* contains a secondary carbohydrate binding site.** Applied Microbiology and Biotechnology, Vol. 100, No. 14, 2016, pp. 6265-6277.
- Wingstrand, Sara Lindeblad; Alvarez, Nicolas J.; Hassager, Ole; Dealy, John M. / **Oscillatory squeeze flow for the study of linear viscoelastic behavior.** Journal of Rheology, Vol. 60, No. 3, 2016, pp. 407-418.
- Yao, Shuo; Lu, Jingquan; Sárossy, Zsuzsa; Baggesen, Claus; Brandt, Anders; An, Yingfeng / **Neutral lipid production in *Dunaliella salina* during osmotic stress and adaptation.** Journal of Applied Phycology, Vol. 28, No. 4, 2016, pp. 2167-2175.
- Yuan, Zhihong; Eden, Mario R.; Gani, Rafiqul / **Toward the Development and Deployment of Large-Scale Carbon Dioxide Capture and Conversion Processes.** Industrial and Engineering Chemistry Research, Vol. 55, No. 12, 2016, pp. 3383-3419.
- Zeng, Zhe; Altarawneh, Mohammednoor; Oluwoye, Ibukun; Glarborg, Peter; Dlugogorski, Bogdan Z. / **Inhibition and Promotion of Pyrolysis by Hydrogen Sulfide ( $H_2S$ ) and Sulfanyl Radical (SH).** The Journal of Physical Chemistry Part A: Molecules, Spectroscopy, Kinetics, Environment and General Theory, Vol. 120, No. 45, 2016, pp. 8941-8948.
- Zeng, Ying; Wang, Ze; Lin, Weigang; Song, Wenli; Christensen, Jakob Munkholt; Jensen, Anker Degn / **Hydrodeoxygenation of phenol over Pd catalysts by in-situ generated hydrogen from aqueous reforming of formic acid.** Catalysis Communications, Vol. 82, 2016, pp. 46-49.
- Zeuner, Birgitte; Nyffenegger, Christian; Mikkelsen, Jørn Dalgaard; Meyer, Anne S. / **Thermostable  $\beta$ -galactosidases for the synthesis of human milk oligosaccharides.** New Biotechnology, Vol. 33, No. 3, 2016, pp. 355-360.
- Zhang, Jianfeng; Liang, Shuai; Yu, Liyun; Skov, Anne Ladegaard; Etmimi, Hussein M.; Mallon, Peter E.; Adronov, Alex; Brook, Michael A. / **Silicone-modified graphene oxide fillers via the Piers-Rubinsztajn reaction.** Journal of Polymer Science. Part A, Polymer Chemistry, Vol. 54, No. 15, 2016, pp. 2379-2385.
- Zhang, Kuiwen; Glarborg, Peter; Zhou, Xueyao; Zhang, Lidong; Ye, Lili; Dayma, Guillaume / **Experimental and Kinetic Modeling Study of Nitroethane Pyrolysis at a Low Pressure: Competition Reactions in the Primary Decomposition.** Energy & Fuels, Vol. 30, No. 9, 2016, pp. 7738-7745.
- Zhang, Lei; Babi, Deenesh Kavi; Gani, Rafiqul / **New Vistas in Chemical Product and Process Design.** Annual Review of Chemical and Biomolecular Engineering, Vol. 7, No. 1, 2016, pp. 557-582.
- Zhang, Yu; Han, Zhennan; Wu, Hao; Lai, Dengguo; Glarborg, Peter; Xu, Guangwen / **Interactive Matching between the Temperature Profile and Secondary Reactions of Oil Shale Pyrolysis.** Energy and Fuels, Vol. 30, No. 4, 2016, pp. 2865-2873.
- Zhou, Guofeng; Jensen, Peter Arendt; Le, Duy M.; Knudsen, Niels O.; Jensen, Anker Degn / **Direct upgrading of fast pyrolysis lignin vapor over the HZSM-5 catalyst.** Green Chemistry, Vol. 18, 2016, pp. 1965-1975.
- Zhou, Guofeng; Jensen, Peter Arendt; Le, Duy Michael; Knudsen, Niels O.; Jensen, Anker Degn / **Atmospheric Hydrodeoxygenation of Biomass Fast Pyrolysis Vapor by  $MoO_3$ .** ACS Sustainable Chemistry & Engineering, Vol. 4, No. 10, 2016, pp. 5432-5440.
- Åberg, Andreas; Widd, Anders; Abildskov, Jens; Huusom, Jakob Kjøbsted / **Estimation of Kinetic Parameters in an Automotive SCR Catalyst Model.** Topics in Catalysis, Vol. 59, No. 10-12, 2016, pp. 945-951.

---

## Books & Monographs

---

- Kontogeorgis, Georgios; Kiil, Søren / **Introduction to Applied Colloid and Surface Chemistry.** 1st edition. Wiley, 2016.
- Seider, Warren D.; Lewin, Daniel R.; Seader, J. D.; Widagdo, Soemantri; Gani, Rafiqul; Ng, Ka Ming / **Product and Process Design Principles: Synthesis, Analysis and Evaluation**, 4th Edition. Wiley, 2016.
- Villadsen, John (Editor); Lee, Sang Yup (series ed.); Nielsen, Jens (series ed.); Stephanopoulos, Gregory (series ed.) / **Fundamental Bioengineering.** Volume 1. Wiley, 2016.

---

## Contributions to books

---

- Babi, Deenesh Kavi; Sales Cruz, Alfonso Mauricio; Gani, Rafiqul / **Fundamentals of process intensification: A process systems engineering view.** Process Intensification in Chemical Engineering: Design Optimization and Control. ed. / Juan Gabriel Segovia-Hernández; Adrián Bonilla-Petriciolet. Springer, 2016, pp. 7-33.
- 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. Vol. 39 Elsevier Science, 2017, pp. 153-196.
- Huusom, Jakob Kjøbsted / **Control of Bioprocesses.** Fundamental Bioengineering. ed. / John Villadsen. Wiley, 2015, pp. 439-462.
- 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. Vol. 39 Elsevier Science, 2017, pp. 61-94.
- Larsen, Morten Andreas Dahl; Drews, Martin; Gani, Rafiqul / **Water consumption in the energy sector.** DTU International Energy Report 2016: The Energy-Water-Food Nexus—from local to global aspects. Technical University of Denmark (DTU), 2016.
- LP Cunico, AK Tula, R Ceriani, R Gani / **Modeling and Prediction of Solid Solubility** by GE Models in Computational Pharmaceutical Solid State Chemistry, Yuriy A Abrahamov (Editor), John Wiley & Sons (chapter 10), 2016, pp. 235-262
- Puig Arnavat, Maria; Bruno, Joan Carles / **Artificial Neural Networks for Thermochemical Conversion of Biomass.** Recent Advances in Thermo-Chemical Conversion of Biomass. ed. / Ashok Pandey; Thallada Bhaskar; M. Stöcker; Rajeev Sukumaran. Elsevier Science, 2015, pp. 133-156.
- Ruiz, Héctor A.; Rodríguez-Jasso, Rosa M.; Aguedo, Mario; Kádár, Zsófia / **Hydrothermal pretreatments of macroalgal biomass for biorefineries.** Algal Biorefineries: Volume 2: Products and Refinery Design. ed. / Aleš Prokop; Rakesh K. Bajpai; Mark E. Zappi. Vol. 2 Springer, 2015, pp. 467-491.
- Sin, Gürkan; Gernaey, Krist / **Data Handling and Parameter Estimation.** Experimental Methods in Wastewater Treatment. ed. / Mark C.M. van Loosdrecht; P.H. Nielsen; C.M. Lopez-Vazquez; Damir Brdjanovic. IWA Publishing Company, 2016, pp. 201-234.
- Skov, Anne Ladegaard (Editor) / **Dielectric Elastomers (DEs) as EAPs: Materials.** Electromechanically Active Polymers. ed. / Federico Carpi. Springer, 2016, pp. 687-714.
- Tonini, Davide; Kougias, Panagiotis; Scheut, Charlotte; Sárossy, Zsuzsa; Thomsen, Tobias Pape; Ahrenfeldt, Jesper; Henriksen, Ulrik Birk; Astrup, Thomas Fruergaard / **Energy recovery from water and food sector residual resources.** DTU International Energy Report 2016: The Energy-Water-Food Nexus—from local to global aspects. ed. / Leif Sønderberg Petersen; Hans Hvidtfeldt Larsen. kgs. Lyngby: Technical University of Denmark (DTU), 2016, pp. 64-72.
- Valverde Pérez, Borja; Flores Alsina, Xavier; Vangsgaard, Anna Katrine; Mauricio-Iglesias, Miguel / **Modelling and control of nitrogen and phosphorus removing systems.** Technologies for the Treatment and Recovery of Nutrients from Industrial Wastewater. IGI global, 2016.





Abu, Rohana/**Process Evaluation Tools for Enzymatic Cascades** Welcome Message.

Alexeev, Artem /**Modeling of Salinity Effects on Waterflooding of Petroleum Reservoirs.**

Anantpinijwatna, Amata/**Generic Model-Based Tailor-Made Design and Analysis of Biphasic Reaction Systems.**

Azizaddini, Seyednezamaddin/**A New Type of Non-Mechanical Valves for Recirculation of Fine Particles.**

Bisgaard, Thomas/**Operation and Design of Diabatic Distillation Processes.**

Bjørner, Martin Gamel/**Thermodynamic modeling of CO<sub>2</sub> mixtures.**

Boiocchi, Riccardo/**Plant-wide modelling and control of nitrous oxide emissions from wastewater treatment plants.**

Chakravarty, Krishna Hara/**Modeling of Salt Solubilities for Smart Water flooding in Carbonate Reservoirs using Extended UNIQUAC Model.**

Gaspar, Jozsef/**CO<sub>2</sub> Capture Dynamic and Steady-State Model Development, Benchmarking, Optimization and Control: Applied to Piperazine and Enzyme Promoted MEA/MDEA.**

Guzman, Jon Trifol/**Hybrid nanocellulose/nanoclay composites for food packaging applications.**

Hansen, Stine Broholm/**Model for Deposition Build-up in Biomass Boilers.**

Hengeller, Ludovica/**Entangled Polymer Melts in Extensional Flow.**

Johansen, Joakim Myung/**Power Plant Burners for Bio-Dust Combustion.**

Kalakul, Sawitree/**Property Model-based Tailor-made Design of Chemical-based Products.**

Kamp, Andreas/**Environmental Sustainability Assessment of Integrated Food and Bioenergy Production with Case Studies from Ghana.**

Khusainova, Aisu/**Enhanced Oil Recovery with Application of Enzymes.**

Larsson, Hilde Kristina/**Modelling of Mass Transfer Phenomena in Chemical and Biochemical Reactor Systems using Computational Fluid Dynamics.**

Liu, Ming/**Pretreatment of hemp fibers for utilization in strong biocomposite materials.**

Manns, Dirk Martin/**Sourcing and bioprocessing of brown seaweed for maximizing glucose release.**

Mansouri, Seyed Soheil/**Integrated Process Design, Control and Analysis of Intensified Chemical Processes.**

Mazurek, Piotr Stanislaw/**Mechanically invisible encapsulations.**

Mears, Lisa/**Novel strategies for control of fermentation processes.**

Narayan, Vikas/**Ash behavior and de-fluidization in low temperature circulation fluidized bed biomass gasifier.**

Nguyen, Hiep Dinh/**Bio-based alkyds by direct enzymatic bulk polymerization.**

Nielsen, Joachim Bachmann/**Valorization of Lignin from Biorefineries for Fuels and Chemicals.**

Nordvang, Rune Thorbjørn /**Production of prebiotic oligosaccharides by novel enzymatic catalysis.**

Papadakis, Emmanouil/**Modelling and synthesis of pharmaceutical processes: moving from batch to continuous.**

Petersen, Thomas/**Model Stickiness in Spray Drying.**

Rasmussen, Helena/**Carbohydrate degradation mechanisms and compounds from pretreated biomass.**

Seita, Catarina Sanches/**Benchmarking of Processes for the Biosynthesis of Natural Products.**

Shabbir, Aamir/**Supramolecular Polymeric Rheology.**

Stolberg-Rohr, Thomine/**Nox Monitoring in Humid Exhaust Gas Using Non-Dispersive Infrared Spectroscopy.**

Trubetskaya, Anna /**Fast pyrolysis of biomass at high temperatures.**

Zakaria, Shamsul Bin/**Electrical Breakdown and Mechanical Ageing in Dielectric Elastomers.**

Zhou, Guofeng/**Simultaneous fast pyrolysis and in situ hydrogenation of lignin to obtain a marine diesel fuel.**







## USEFUL INFORMATION

### **Automation**

An automated liquid handling workstation gives a high throughput evaluation of engineered enzymes in the laboratory of the BioEng research centre

Photo: Thorkild Christensen

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

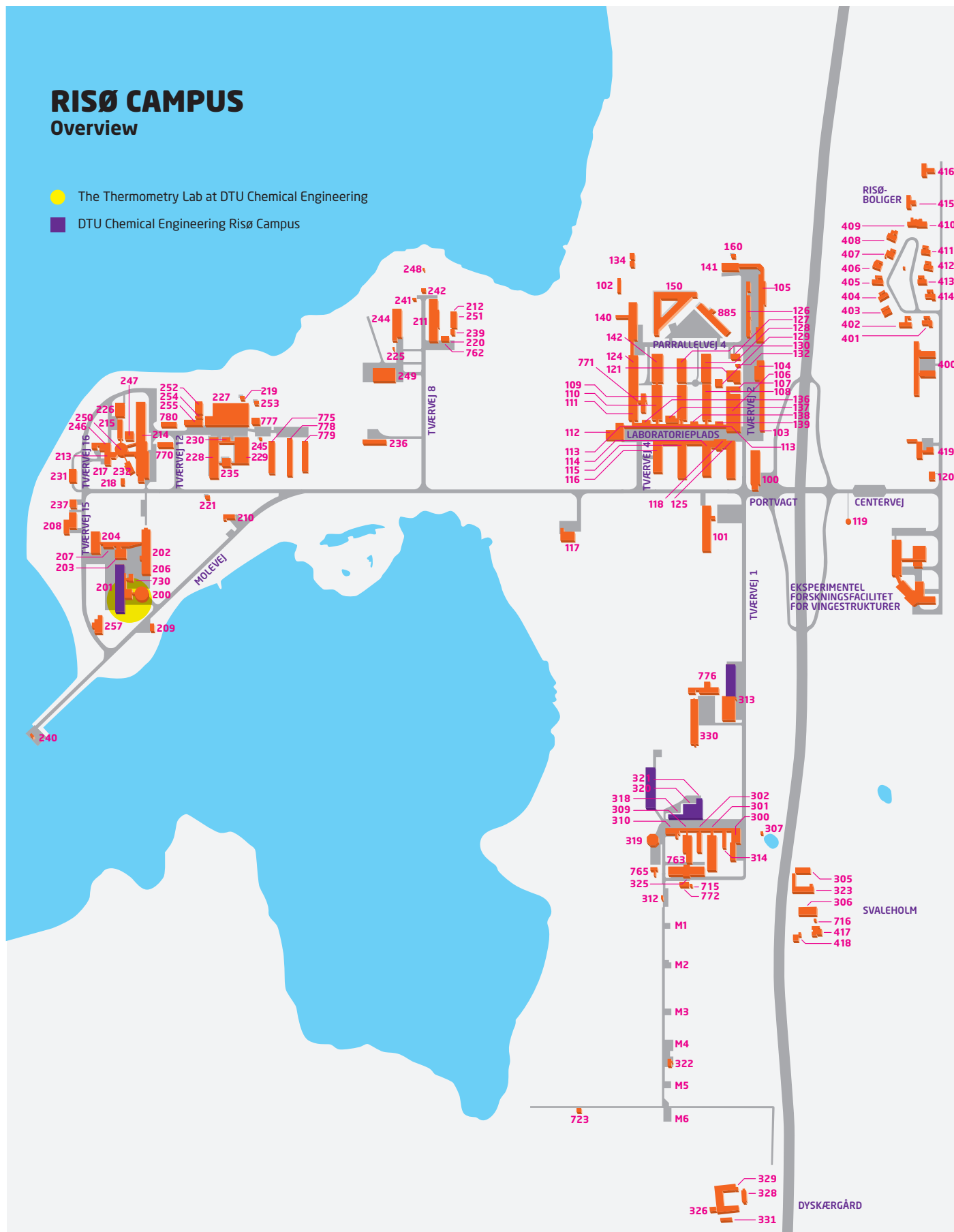


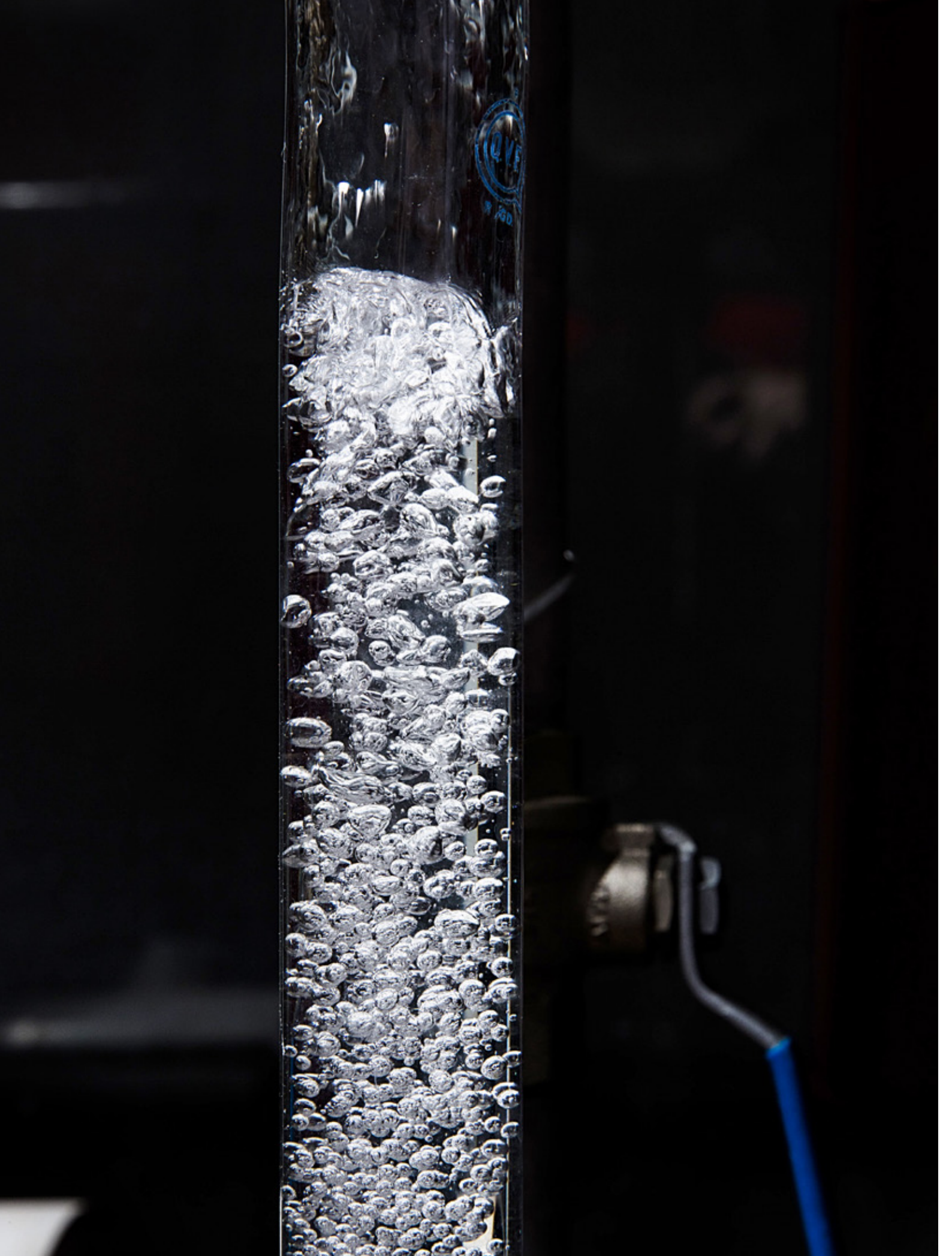


# RISØ CAMPUS

## Overview

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







**Department of Chemical and Biochemical Engineering**  
Technical University of Denmark  
DK-2800 Kgs. Lyngby  
Denmark

Phone +45 4525 2800  
Fax +45 4588 2258  
E-mail [informationen@kt.dtu.dk](mailto:informationen@kt.dtu.dk)  
Web [www.kt.dtu.dk](http://www.kt.dtu.dk)

**Annual Report 2016**

February 2017

ISBN-13: 978-87-93054-78-3

Department of Chemical and Biochemical Engineering  
Technical University of Denmark  
DK 2800 Kgs. Lyngby, Denmark

**Editor in chief**

Professor Kim Dam-Johansen, Head of Department

**Editing, project management & articles**

Lotte Grandorf, Communications Officer

**With great support from student workers**

Frederik Appel Olsen & Ausrine Kriucokaite

**Photos**

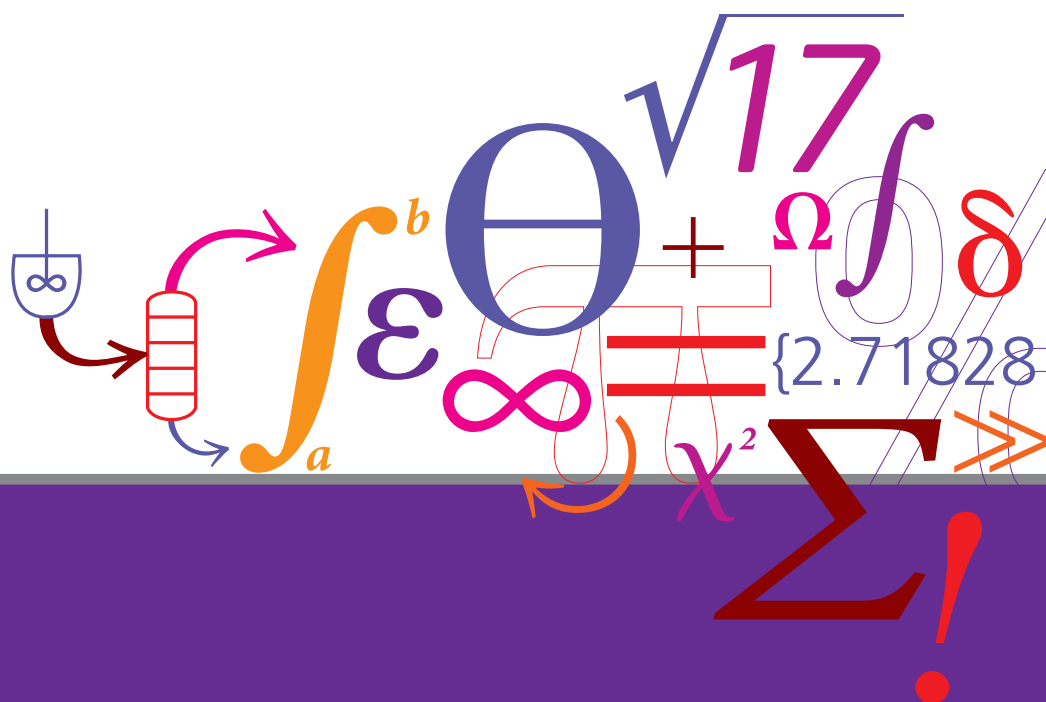
Thorkild Christensen, unless stated otherwise

**Design & production**

STEP

**Print**

STEP



This Annual Report 2016 may be ordered from the reception at the  
Department of Chemical and Biochemical Engineering, DTU  
Phone +45 4525 2800

E-mail [informationen@kt.dtu.dk](mailto:informationen@kt.dtu.dk)

Also available on [www.kt.dtu.dk](http://www.kt.dtu.dk)

Follow DTU Chemical Engineering on

**LinkedIn**

[www.linkedin.com/company/398282](http://www.linkedin.com/company/398282)

