

**Program for CERE Discussion Meeting
18-20 June 2018**

Hotel Rungstedgaard, Rungsted Kyst, Denmark

Monday, 18 June

- 09:30 - 11:00** Demonstration of the Experimental Facilities of CERE with rolling presentation and relevant posters (*Nicolas von Solms, Tobias Orlander*), Lab Tour (*Nicolas von Solms*) and Demonstration of the Virtual Reality Room (VR) (*Wei Yan*)
- 11:15** Departure by bus from DTU Chemical Engineering to Hotel Rungstedgaard
- 12:00 - 13:00** **Lunch**
- 13:00 - 13:10** Welcome and News by Georgios M. Kontogeorgis

Plenary Lectures Session – 1 (*Georgios M. Kontogeorgis*)

- 13:10 - 13:30** The Gas Hydrate Project 2007-2017
(*Nicolas von Solms*)
- 13:30 - 13:50** Overview of the OPTION project – towards completion
(*Erling H. Stenby*)
- 13:50 - 14:15** Scientific Computing using Advanced Simulation Technologies
(*Allan Peter Engsig-Karup*)
- 14:15 - 14:40** Petrography and stratigraphy of the Lower Cretaceous succession
(*Thomas G. Petersen, new faculty in CERE*)
- 14:40 - 15:00** Water Research at CERE – Status and some personal thoughts
(*Georgios M. Kontogeorgis*)
- 15:00 - 15:30** **Coffee Break**
- 15:30 - 18:00** **Parallel Sessions 1 & 2**

Parallel Session 1: Thermodynamics – CHIGP and more (*Xiaodong Liang*)

- 15:30 - 15:50** The Subsea factory: measurements and modelling for remote process design
(*Francois Kruger*)
- 15:50 - 16:10** Use of natural variables to solve state function based flash problems
(*Duncan Paterson*)

Parallel Session 2: Simulation and Optimization-I (*John Bagterp Jørgensen, & Wei Yan*)

- Nonlinear Model Predictive Control of UV Flash Processes (*Tobias Kasper Skovborg Ritschel*)
- A Least Squares Method for Ensemble-based Multi-objective Oil Production Optimization
(*John Bagterp Jørgensen*)

16:10 - 16:30	Calculation of Adsorption and Interfacial Tension with Classical Density Functional Theory (<i>Edgar Vergara</i>)	Phase envelope in the presence of capillary pressure calculated using volume-based thermodynamics (<i>Diego Sandoval</i>)
16:30 - 16:50	Application of the crossover approach with cubic and CPA equations of state (<i>Andre Vinhal</i>)	Application of non-stoichiometric CPE algorithms to geochemical multiphase reactions (<i>Christos Tsanas</i>)
16:50 - 17:10	A review of the asphaltene modeling work (<i>Alay Arya</i>)	Multiphase coupling of reservoir simulator and computational fluid dynamics (<i>Casper Schytte Hemmingsen</i>)
17:10 - 17:30	Renormalization Group Theory in Phase Equilibria Modelling: Applications with Cubic Equations of State (<i>Gabriel Silva</i>)	Use of (T,V) variables to rapidly solve isothermal flash problems for complex equations of state dynamic simulation (<i>Duncan Paterson</i>)
17:45 – 18:45	CERE Member Companies Round Table Discussion	
19:00	Dinner	

Tuesday, 19 June

Plenary Lectures Session – 2 (*Alexander Shapiro*)

- 08:15 - 08:30 Overview of the EOR projects (*Alexander Shapiro*)
- 08:30 - 09:00 Technology maturation in DHRTC (*Hans Horikx, DHRTC*)
- 09:00 - 09:30 Solving large-scale computational problems in geoscience (*Klaus Mosegaard, Niels Bohr, Copenhagen University*)
- 09:30 - 10:00 Industrial Presentation by Welltec: Risk management in field development (*Mette Lind Fürstnow*)
- 10:00 - 10:30 Coffee Break**

Parallel Sessions 3 & 4

Parallel Session 3: Petroleum Applications (*Alexander Shapiro, Ida Fabricius*)

Parallel Session 4: Ionic liquids and more (*Philip Fosbøl, Kaj Thomsen*)

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| 10:30 - 10:50 | Temperature effects on the effective stress field in the deep North Sea Basin (<i>Tobias Orlander</i>) | The SULCOR project-Corrosion measurements (<i>Henrik Lund Nielsen</i>) |
| 10:50 - 11:10 | Elastic moduli, stiffness and effective stress of chalk from Zealand and from Dan field (North Sea) (<i>Laura Paci</i>) | Thermodynamic Modeling of Dissociation Conditions of Semi-clathrate Hydrates of Tetra-n-butyl Ammonium Halides Using Electrolyte CPA Equation of State (<i>Li Sun</i>) |
| 11:10 - 11:30 | Extended PVT study of high pressure-high temperature reservoir fluids including the reverse Joule-Thomson effect (<i>Teresa Regueira Muniz</i>) | Properties of multifunctional ionic liquid VAIMTFSI ((1-vinyl-3-acetamido imidazole bis(trifluoromethylsulfonyl) imide in binary and ternary mixtures for lithium batteries (<i>Yingjun Cai</i>) |
| 11:30 - 11:50 | Prediction of downhole scaling using thermodynamic calculations and production (<i>Ida Arent Kirknel</i>) | Efficient Transformation of Atmospheric CO ₂ to Carbonates by DBU Based Ionic Liquids under Mild Conditions (<i>Xianglei Meng</i>) |
| 11:50 - 12:10 | Experimental study of high-pressure phase equilibrium and density of asymmetric mixtures related to reservoir fluids (<i>Yiqun Liu</i>) | Water Bridging Initiative - from descaling drinking water to disarming resistant microbes (<i>Nikolaj Blom</i>) |
| 12:10-13:00 | Lunch (joined with KT-Consortium staff and industrial representatives) | |

Parallel Sessions 5, 6 & 7

Parallel Sessions 5 & 6

Parallel Session 5: SYNFERON project (*Georgios M. Kontogeorgis/Ioannis Skiadas*)

Parallel Session 6: DHRTC collaborations (*Alexander Shapiro, Ida Fabricius*)

13:00-13:20	WP1: The biomass gasifier for syngas production (<i>Niels Bjarne K. Rasmussen</i>)	Software for Industrial Scale Oil Production Optimization (<i>Steen Hørsholt</i>)
13:20-13:40	WP2: Syngas biomethanation by mixed microbial consortia in anaerobic trickle bed reactors (<i>Konstantinos Asimakopoulos</i>)	Failure characterization in geomechanical testing using Nuclear Magnetic Resonance spectroscopy (<i>Leonardo Teixeira Pinto Meireles</i>)
13:40-14:00	WP2: Mixed microbial cultures for syngas fermentation to ethanol and methane (<i>Antonio Grimalt Alemany</i>)	Gas injection and phase behavior in tight Lower Cretaceous reservoirs (<i>Wei Yan</i>)
14:00-14:20	WP2: Analysis of microbial mixed cultures, (incl. both organismal composition and mapping of functional genes), seen in perspective of their metabolic potential (<i>Lene Lange</i>)	Fluid-rock interactions and their impacts on oil recovery during SmartWater injection in chalk reservoirs (<i>Jiasheng Hao</i>)
14:20-14:50	Coffee Break	Coffee Break
14:50-15:10	WP3: Advanced Downstream Processing Systems (<i>Jens Abildskov</i>)	Mobilizing oil with nanoparticles (<i>Muhammad Waseem Arshad</i>)
15:10-15:30	WP4: Simulation of energy consumption in bio-product recovery from syngas fermentation (<i>Mauro Torli</i>)	Sulfide Scales Solubility at High Temperatures using Extended UNIQUAC (<i>Diana Carolina Figueroa Murcia</i>)
15:30-15:50	General Technical Discussion	Forward modeling of deposition and consolidation of sedimentary rocks (<i>Ivanka Bekkevold</i>)

Parallel Session 7

ICAS and CERE software Workshop (*Xiaodong Liang, Alay Arya, Kaj Thomsen, Spardha Jhamb and Nipun Garg*)

13:00 - 13:10	Introduction and overview of ICAS (<i>Xiaodong Liang</i>)
13:10 - 13:30	Pure component properties and models: Database Manager and ProPred (<i>Alay Arya</i>)
13:30 - 13:55	ProCAMD (Computer Aided Molecular Design) / VPPD Lab (<i>Spardha Jhamb</i>)
13:55 - 14:15	SolventPro (Solvent Selection and Design Framework) (<i>Xiaodong Liang</i>)

14:15 - 14:35	Coffee break
14:35 - 15:05	Super-O: Superstructure Optimization & SustainPro, LCSOft (Nipun Garg)
15:05 - 15:20	ThermoSystem: CPA in simulators (Alay Arya)
15:20 - 15:35	Scale-CERE: Extended-UNIQUAC applications (Kaj Thomsen)
15:35 - 15:50	CPA and PC-SAFT in MATLAB (Xiaodong Liang)

16:00-18:30 **Joint CERE and KT-Consortium Poster Session**

CERE Posters (three awards – votes by CERE industrial members)

Oil & Gas – Petroleum Applications, CO₂-related applications

C-1 *Jyoti Shanker Pandey: Molecular scale experiments of hydrate swapping processes*

C-2 *Jyoti Shanker Pandey: Cavity driven acid placement & workhole propagation in chalk reservoir: Deeper acid penetration & efficient jetting*

C-3 *Meng Shi: Flue gas injection and depressurization of natural gas hydrate for CH₄ recovery and CO₂ storage*

C-4 *Einar Madsen Storebø: Lower Cretaceous tight reservoir permeability modeling*

C-5 *Amirali Rezzazadeh: New promoted concepts for reducing energy consumption in CO₂ capture amine solutions*

C-6 *Randi Neerup: BioCO₂ – A CERE project on biogas upgrading*

C-7 *Mick Kolster: Magnetic survey for UXO detection in an onshore setting with external long wavelength disturbances*

C-8 *Wael Almasri: Gas Liberation in Tight Permeable Reservoirs*

C-9 *Casper Schytte Hemmingsen: Completion evaluation with computational fluid dynamics*

C-10 *Samira Mohammadkhani: Smart waterflooding with bicarbonates*

C-11 *Wojciech Laskowski: Multigrid acceleration of a spectral element solver for marine hydrodynamics*

C-12 *Jacob Hicks: Development of a potential flow solver including wave-structure interaction*

C-13 *Aikaterini Zeneli: Petrophysical interpretation of the Lark formation*

C-14 *Carsten Völcker: Near-wellbore modeling in ECLIPSE with Computational Fluid Dynamics*

C-15 *Yuntian Teng: Experimental study of adding nanocellulose into the injection water for possible EOR*

Property Predictions and Thermodynamics

(these posters will also participate in the KT-Consortium poster award competition)

- J-7** Kai Kang: Estimation of thermodynamic derivative properties of Hydrofluoroolefins (HFOs) using PC-SAFT and CPA Equation of State
- J-8** Kai Kang: Estimation of thermodynamic derivative properties of *n*-decane with *p*-xylene, *m*-xylene and *o*-xylene binary mixtures using PC-SAFT and CPA Equation of State
- J-9** Asma Rafsanjani: Comparison of crossover theories for the prediction of critical point of hydrocarbons
- J-10** Jiahuan Tong: A Novel Coarse-grained Model for 1-alkyl-3-methyl-imidazolium Chloride Ionic Liquids
- J-11** Athanasios Antonios Varsos: Thermodynamics of petroleum fluids relevant to subsea processing
- J-12** Andre Vinhal: Application of the cross-over approach with cubic and CPA equations of state
- J-13** Mauro Torli: Simulation of energy consumption in bio-product recovery from syngas fermentation
- J-14** Edgar Vergara: Calculation of Adsorption and Interfacial Tension with Classical Density Functional Theory
- J-15** Li Sun: Thermodynamic Modeling of Dissociation Conditions of Semi-clathrate Hydrates of Tetra-*n*-butyl Ammonium Halides Using Electrolyte CPA Equation of State
- J-16** Francois Kruger: Implications of new multicomponent phase equilibrium data for the design of subsea natural gas dehydration facilities
- J-17** Xianglei Meng: Biological porphyrin ionic liquids as photocatalysts for conversion of CO₂ to carbonates at mild conditions
- J-19** Michael Bache: Investigation of an ultrasound device used for CaCO₃ descaling of drinking water

J-C de Hemptinne, P. Mougin: Electrolyte Thermodynamics Joint Industrial Project
(Poster by a CERE member company)

KT-Consortium Posters (one award – votes by KT-Consortium members)

(posters marked with * will also participate in the CERE poster award competition)

- J-1** Martin Due Olsen: Thermodynamic modeling of the solubility of pharmaceuticals with PC-SAFT*
- J-2** Xinyan Liu: Property Modeling of Ionic Liquids for Gas Separation Processes*
- J-3** Spardha V. Jhamb: Substitution from Chemical-based Products using a Model-based Methodology*
- J-4** Yuqiu Chen: Ionic liquid (IL) database development*
- J-5** Olivia Ana Perederic: Systematic methods and tools for lipids process technology*
- J-6** Saeed Eini: Developing group contribution models for the Atmospheric Lifetime and Minimum Ignition Energy*
- J-18** Alay Arya: Recent application of CPA for flow assurance (asphaltenes)*
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- K-1** *Nima Nazemzadeh: Molecular Tracking: An Alternative Computer-Aided Concept for Multi-Component Distillation Column Design*
- K-2** *Giorgio Colombo: Rapid and efficient development of downstream processing alternatives for biopharmaceutical processes*
- K-3** *David Sargis Hambartsumyan: Optimization-based Integrated Product-Process Design – Application on Acetic Acid/Water Extraction*
- K-4** *Beatrice Mazzali: Systematic Decision-Support Framework for Efficiently Achieving Resource Recovery in Bio-based Industry*
- K-5** *Dominic Andrew Silk: Systematic techno-economic decision framework for resource recovery*
- K-6** *Simoneta Caño de Las Heras: A holistic methodology for development of a pedagogical simulation tool used in fermentation applications*
- K-7** *Rasmus Fjordbak Nielsen: Integrated Process Design and Control of Intensified Chemical Processes: Case Study of Periodic Reactive Distillation*
- K-8** *Louise la Cour Freiesleben: Periodic Separation Process Intensification*
- K-9** *Nipun Garg: A multi scale and multi-level computer aided approach for Process Intensification*
- K-10** *Hongliang Qian: Exergy efficiency based design and analysis of utilization pathways of biomasses*
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19:00 Aperitif

19:30 Joint Gala Conference Dinner for CERE & KT-Consortium – After Dinner Talk
(DTU Provost Rasmus Larsen)

Award Ceremonies for Posters from CERE and KT-Consortium

Wednesday, 20 June (Joint CERE and KT-Consortium Day)

Plenary Lectures Session – 3: Joint CERE and KT-Consortium Session (*Georgios M. Kontogeorgis*)

- 08:40 - 08:50** CERE & KT-Consortium: Two centers, two consortia but much in common
(*Georgios M. Kontogeorgis*)
- 08:50 - 09:05** Software in CERE and Software in KT-Consortium (ICAS) – A short introduction
(*Alay Arya, Xiaodong Liang, Nipun Garg*)
- 09:05 - 09:20** Experimental activities in CERE (*Nicolas von Solms, Wei Yan and Ida Fabricius*)
- 09:20 - 09:40** Thermodynamics, simulation, control, optimization, and scientific computing
(*John Bagterp Jørgensen*)
- 09:40 - 10:00** The need for property prediction and thermodynamic data for biological conversions
(*John Woodley*)
- 10:00 - 10:30** **Invited lecture by Professor John O’Connell:** Analysis of chemical process systems with explicit accounting for entropy generation
- 10:30 - 11:00** **Coffee Break**
- 11:00 - 11:30** **Industrial presentation by a CERE member company**
(*BP/Dr. Nikos Diamantonis*) Physical properties in different stages of process development
- 11:30 - 12:00** CERE Discussion Meeting – Closing remarks (*Georgios M. Kontogeorgis*)
- 12:00 - 13:00** **Lunch (both centers/consortia)**
- 13:30** Departure by bus to DTU Chemical Engineering (optional)
- 13:00 - 15:00** Possibility to attend the following joint KT-Consortium & CERE program
- Chair: Xiaodong Liang*
- 13:00 - 13:30** **Invited lecture by Dr. Ioannis Tsivintzelis (Aristotle University of Thessaloniki):**
Phase Equilibria for biodiesel-related compounds with CPA
- 13:30 - 13:50** *PhD student Olivia Ana Perederic*
Phase equilibria modelling applied to design and analysis of a lipids related process
- 13:50 - 14:20** *Assistant Professor Xiaodong Liang:* On the PT Flash calculations with equations of state
- 14:20 - 14:40** *PhD student Spardha V. Jhamb*
A General, Model-based Methodology for Chemical Substitution
- 14:40 - 15:00** *Guest PhD student Saeed Eini*
Multi-objective optimization of an LNG process
- 15:00 - 15:20** *PhD student Francois J. Kruger*
Towards Practical Application of Uncertainty Analysis in Process Design and Monitoring
- 14:15 - 17:00** Individual Meetings