



Program for CERE Discussion Meeting 11-13 June 2019 Beach Hotel Marienlyst, Denmark

Tuesday, 11 June

- 09:30-11:00** Demonstration of Experimental Facilities of CERE with rolling presentation and relevant posters (*Nicolas von Solms, Tobias Orlander*), Lab Tour (*Nicolas von Solms*)
- 11:15** Departure by Bus from DTU Chemical Engineering to Hotel Marienlyst
- 12:00-13:00** **Lunch**
- 13:00-13:05** Welcome and News by Georgios M. Kontogeorgis

Plenary Lectures Session – 1 (*Georgios M. Kontogeorgis*) (Kronborg 1+2)

- 13:05-13:35** Overview of the OPTION project – Integration and Optimization of Oil Reservoir Operation (*John Bagterp Jørgensen*)
- 13:35-14:05** **Geothermal energy – How to unlock this large, green and renewable energy source, Industrial presentation by Susanne Poulsen, A.P. Møller Holding A/S**
- 14:05-14:30** Modeling of PbCl_2 solubility in brines (*Kaj Thomsen*)
- 14:30-15:00** Overview of the CCS activities of CERE (*Philip L. Fosbøl*)
- 15:00-15:30** **Coffee Break**
- 15:30-18:00** **Parallel Sessions 1 & 2**

(Seaside)

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

(Kronborg 1+2)

Parallel Session 2: CO₂ capture and Electrolytes (*Philip Fosbøl*)

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| 15:30-15:50 | Advances in the Implementation of Classical Density Functional Theory in the study of Inhomogeneous Systems (<i>Edgar Camacho Vergara</i>) | Biological solvents for carbon capture (<i>Humbul Suleman</i>) |
| 15:50-16:10 | Compositional reservoir simulation and flash algorithms (<i>Duncan Paterson</i>) | Test Center Mongstad CO ₂ pilot tests focused at energy reduction (<i>Randi Neerup</i>) |
| 16:10-16:30 | Applications of non-stoichiometric multiphase reaction algorithms (<i>Christos Tsanas</i>) | Biogas Desulfurization within the MeGa-StoRE Project (<i>Sebastian Nis Bay Villadsen</i>) |
| 16:30-16:50 | Properties and thermodynamics on regenerating plastic (<i>Amirali Rezazadeh</i>) | Synthesis of a novel type of ionic liquid and its application in lithium batteries (<i>Yingjun Cai</i>) |
| 16:50-17:10 | The WaterStruc project (<i>Johan Kronholm</i>) | Modeling of gas solubility in aqueous electrolyte solutions using the Electrolyte Cubic-Plus-Association Equation of State (<i>Li Sun</i>) |
| 17:10-17:30 | Water Bridging Initiative – applications of a new science of water (<i>Nikolaj Blom</i>) | Scale solubility in CO ₂ corrosion (<i>Carolina Figueroa</i>) |

17:35-18:45 CERE Member Companies Round Table Discussion (Kronborg 8)

17:35-17:55 *Thermodynamics (Georgios Kontogeorgis)*

17:55-18:15 *CCUS (Erling H. Stenby)*

18:15-18:35 *Reservoir Engineering (Ida Lykke Fabricius)*

18:35-18:45 *Any other topic (Alexander Shapiro)*

19:00 Dinner

Wednesday, 12 June

Plenary Lectures Session – 2 (Alexander Shapiro) (Kronborg 1+2)

08:15-08:40 Overview of the SmartWater project (*Alexander Shapiro*)

08:40-09:05 Electrolytes and geological material (*Ida Fabricius*)

09:05-09:30 Modeling and simulation of gas injection in tight formation (*Wei Yan*)

09:30-10:00 **Linking up Pressure, Compositional and Thermal Gradients, Invited presentation by François Montel, University of Pau**

10:00-10:30 **Coffee Break**

Parallel Sessions 3 & 4

(Seaside)

Parallel Session 3: Petroleum Applications/DHRTC-1 (Alexander Shapiro, Ida Fabricius)

10:30-10:50 Gas liberation in porous medium. Experiment and modeling (*Wael Al-Masri*)

10:50-11:10 Study of fluid distribution in a tight petroleum reservoir (*Hadise Baghooee*)

11:10-11:30 Microfluidics studies of motion of oil drops in thin capillaries (*Tian Wang*)

11:30-11:50 Chalk stiffness: Distribution in the Maastrichtian unit of the Dan Field (*Leonardo Teixeira Pinto Meireles*)

11:50-12:10 Phase Equilibria Studies Relevant to Natural Gas Subsea Processing: Experimental VLLE studies for Natural Gas related mixtures (*Athanasios Varsos*)

12:10-13:00 **Lunch (joined with KT-Consortium staff and industrial representatives)**

(Kronborg 1+2)

Parallel Session 4: CO₂ storage and underground processes (Nicolas von Solms, Wei Yan)

Multilayer hydrate sediment gas production behavior by depressurization with CO₂-enriched air (*Meng Shi*)

Kinetics of CH₄-CO₂ exchange in different mass transfer scenarios (*Jyoti Shanker Pandey*)

Calculation of geochemical reactions in CO₂ EOR/sequestration processes (*Fernando Medeiros*)

Chalk dissolution: Understanding what we see (*Yi Yang*)

Phase equilibrium and density of highly asymmetric gas-oil mixtures at high temperatures and high pressures (*Yiqun Liu*)

Parallel Sessions 5, 6 & 7

Parallel Sessions 5 & 6

	(Kronborg 1+2) Parallel Session 5: SYNFERON project <i>(Ioannis Skiadas)</i>	(Seaside) Parallel Session 6: DHRTC collaborations-2 <i>(Alexander Shapiro, Ida Fabricius)</i>
13:00-13:20	WP1: From wood to biogas – a small scale demonstration (<i>Niels Bjarne K. Rasmussen</i>)	Thermal stress in the effective stress equation (<i>Tobias Orlander</i>)
13:20-13:40	WP2: Syngas biomethanation in a trickle bed reactor (<i>Konstantinos Asimakopoulos</i>)	Modelling permeability and capillary pressure for Lower Cretaceous marly chalks (<i>Einar Storebø</i>)
13:40-14:00	WP2: Mixed microbial culture-based syngas fermentation (<i>Antonio Grimalt Alemany</i>)	Nanoparticles for EOR (<i>Muhammad Wassem Arshad</i>)
14:00-14:20	WP3: Advanced Downstream Processing Systems - Overview (<i>Jens Abildskov</i>)	Experimental study of the porous media effects on phase behavior (<i>Teresa Regueira Muniz</i>)
14:20-14:40	WP4: Benchmarking syngas fermentation purification technologies (<i>Mauro Torli</i>)	Simulation of oil production from tight formation (<i>Diego Sandoval</i>)
14:40-15:00	Biotransformations of syngas within SYNFERON: an overview of applications potential (<i>Hariklia Gavala</i>)	Forward Modelling of Geopressures in the Central Graben (<i>Ivanka Orozova-Bekkevold</i>)

Parallel Session 7 (Kronborg 8)

ICAS software Workshop

(Xiaodong Liang, Edgar Camacho Vergara, Nipun Garg, Spardha V. Jhamb, and Simoneta Caro de las Heras)

13:00-13:05	Open the session and introduction (Xiaodong Liang)
13:05-13:30	Overview of ICAS, ProPred, Database manager, and AzeroPro (Edgar L. Camacho Vergara)
13:30-13:55	Computer-Aided Product Design Tools: Pro-CAMD and VPPDlab (Spardha Jhamb)
13:55-14:20	Super-O (Superstructure Optimisation), SustainPro & LCSOFT (Nipun Garg)
14:20-14:40	Development of a Virtual Educational BioProcess (Simoneta Cano de las Heras)
14:40-15:00	Interfaces to CPA and PC-SAFT codes and close the session (Xiaodong Liang)
15:00-15:15	Coffee Break – Group picture at the terrace outside Seaside/Kronborg
15:15-15:30	EleTher JIP : an industrial community on Electrolyte Thermodynamics, by Jean-Charles de Hemptinne, IFP Energies Nouvelles
15:30-16:15:	Short video presentations of posters (in plenum) (Kronborg 1+2)

16:15-18:30 Joint CERE and KT-Consortium Poster Session (Kronborg 1+2, Seaside & Kronborg Hall)

CERE Posters (Two awards, one for Thermodynamics/CCS and one for Petroleum and Related Applications – votes by CERE industrial members)

Oil & Gas – Petroleum and Related Applications

- C01** Yibo Yang: *Molecular diffusion of reservoir fluid systems in porous media*
- C02** Zahra Nickman: *Extend Coiled Tubing Reach Using Polymers as Friction and Viscosity Reducers*
- C03** Jiasheng Hao: *Effect Of Compaction On Oil Recovery Under Low Salinity Flooding In Homogeneous And Heterogeneous Chalk*
- C04** Ermis Proestakis and Leonardo Meireles: *Optimization of single salt brine composition characterized by potential determining ions for maximizing water weakening in Stevns Klint chalk*
- C05** Marco Collura and Tobias Orlander: *Effects of high temperature core flooding on stiffness properties of Gassum sandstone*
- C06** Einar Storebø: *Modelling permeability and capillary pressure curves for Lower Cretaceous marly chinks*
- C07** Maria del Pilar Clemente Vidal: *Sequence stratigraphy of extensional continental basins and petroleum geology*
- C08** Ivanka Orozova-Bekkevold: *Forward Modelling of Geopressures in the Central Graben*
- C09** Natalia Krygier & Ivanka Orozova Bekkevold: *Non Productive Time (NPT) while drilling with regards to well stability issues*
- C10** Fernando Reyes Gonzales & Ivanka Orozova-Bekkevold: *Wellbore stability around salt bodies: A Case Study for the Oselvar field in the North Sea*
- C11** Kianoosh Moeini: *Geothermal energy production and heat storage potential of the Frederikshavn formation*
- C12** Arne Døssing Andreassen: *Development and application of UAV based energy and mineral exploration systems*

Property Predictions, Thermodynamics and CCS

(with * those that participate also in the KT-Consortium poster award competition)

- C13** Daniel Qvistgaard*: *Thermodynamic Modelling of Associating Compounds for Gas Processing*
- C14** Meng Shi: *Multilayer hydrate sediment gas production behavior by depressurization with CO₂-enriched air*
- C15** Jyoti Shanker Pandey: *Kinetics of CH₄-CO₂ exchange in different mass transfer scenarios*
- C16** Jing Cai: *Thermodynamic Modelling of gas hydrates for CCUS applications*
- C17** Randi Neerup: *Test Center Mongstad CO₂ pilot tests focused at energy reduction*
- C18** Lucas Corrêa: *CO₂ capture in a new solvent mixture*
- C19** Sai Hema Bhavya Vinjarapu: *Ultrasound assisted desorption of CO₂ from MEA*
- J01** Xianglei Meng*: *Aluminum-containing Ionic Liquid for Cycloaddition of CO₂ with Epoxides under Mild Conditions*
- J02** Jiahuan Tong*: *Structural and dynamic properties of high concentration lithium containing solutions*
- J03** Francois Kruger*: *New Multicomponent Phase Equilibrium Data for the Design of Subsea Natural Gas Dehydration Facilities*

- J04** Athanasios Varsos*: *Experimental VLE studies for natural gas related mixtures*
- J05** Li Sun*: *Modeling of Gas Solubility in Aqueous Electrolyte Solutions using the Electrolyte Cubic-Plus-Association Equation of State*
- J06** Li Sun*: *Thermodynamic Study on Ionic Liquid-Water as Alternative Working Pairs for Absorption Refrigeration Cycle*
- J07** Edgar Vergara*: *Modelling of Asphaltene Adsorption with Advanced Molecular Models: A Classical DFT Approach*
- J08** Mauro Torli*: *CFD simulation study of mass transfer performance in a bubble column for applications in syngas fermentation*
- J09** Michael Bache*: *Spectroscopic investigations on water hydrogen bond formation in electrolyte solutions*
- J10** Nomiki Kottaki*: *Experimental investigation on the floating water bridge phenomenon*
- J11** Asma Jamali Rafsanjani*: *Prediction of Second Order Derivative Properties of Selected n-Alkanes through two Different Renormalization Group Methods*

KT-Consortium Posters (one award – votes by KT-Consortium members)
(with * those that participate also in the CERE poster award competition under “Thermodynamics/CCS”)

- J12** Xinyan Liu*: *Ionic liquid screening for shale gas separation*
- J13** Spardha Jhamb*: *Solvent Selection for Coatings Formulation: Method, Applications and Issues*
- J14** Spardha Jhamb & Irene Hospital*: *A Group Contribution Model to Predict the Biodegradability of Organic Compounds*
- J15** Yuqiu Chen*: *Ionic liquid design and process simulation for separation of aqueous solutions*
- J16** Markus Enekvist*: *Property estimation and database of pigment properties for paint design*
- J17** Olivia Ana Perederic*: *Systematic Computer Aided Methods and Tools for Lipid Process Technology*
- K01** Rowan Malan Lindeque: *Thermodynamic Property Prediction for Biocatalysis with Q-props*
- K02** Mark Jones: *A Modular and Multi-scale Modelling Framework for Computer-Aided Process Design and Optimisation*
- K03** Simoneta Caño de Las Heras: *Development of Pedagogically Tailored Bioprocess Simulators*
- K04** Nipun Garg: *Phenomena based synthesis-intensification: generalized method and case studies*
- K05** Abhimanyu Pudi: *Integration of Process Systems Engineering & Computational Chemistry for Process Intensification*
- K06** Adam Paul Karcz: *Integration of Process Design and Computational Chemistry for Process Intensification*
- K07** Vahid Shadravan: *Sour Gas Sweetening via Catalytic H₂S Conversion: An Innovative Intensified Solution*
- K08** Enrico Mancini: *Sustainable and cost-effective downstream routes for separation of bio-succinic acid*
- K09** Nikolaus Vollmer: *Sustainable value chain design for biorefineries*

- K10** Philip Heldt Sørensen & Binoy Hasmukh Shah: *Modelling and design of the Downstream Processing (DSP) for the Biotechnological Production of Xylitol*
- K11** Nicklas Leander Lund: *Systematic Downstream Process Synthesis, Design and Analysis for Butanol Production*
- K12** Frederico C.C. Montes: *Data-driven Control for Batch Crystallization Processes*
- K13** Merve Öner: *Validation of a Pilot Scale Pharmaceutical Crystallization Process Model*
- K14** Anders Jakobsen: *Synergistic Combination of Two-stage Fermentation and in-situ Product Removal in the Production of Biochemical*
- K15** Ergys Pahija: *Sequential Monte Carlo to model Lactic Acid Bacteria Fermentation*
- K16** Atli Freyr Magnusson: *Optimization of parametric uncertain designs using a novel stochastic optimization methodology*
- K17** Martina Alvarez Camps: *Dynamic Control of a Methanol Refining Wall Column*
- K18** Andreas Nørgreen: *A Digital Twin for CAPS - Capacity Analysis, Production Planning & Scheduling*

19:00 **Aperitif and live music (Terrace on the Seaside)**

19:30 Joint Gala Conference Dinner for CERE & KT-Consortium

Award Ceremonies for Posters from CERE (One for Thermodynamics/CCS, one for Petroleum and related Applications) and one from KT-Consortium

Thursday, 13 June (Joint CERE and KT-Consortium Day)

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

08:40-08:45	CERE & KT-Consortium: Welcome, Introduction to the two consortia and common program of the day (<i>Georgios M. Kontogeorgis</i>)
08:45-09:00	Software at CERE and Software at KT-Consortium (ICAS) – A short introduction (<i>Edgar L. Camacho Vergara and Xiaodong Liang</i>)
09:00-09:15	Experimental activities at CERE (<i>Nicolas von Solms, Wei Yan and Tobias Orlander</i>)
09:15-09:50	Industrial Presentation by a member company – 1: A topology-based dispersion activity coefficient model derived from PC-SAFT (<i>Gerard Krooshof, DSM</i>)
09:50-10:25	Industrial Presentation by a member company – 2: How can we promote Digital Transformation in Mitsubishi Chemical Corporation? (<i>Koutaro Ouchida, Mitsubishi Chemicals</i>)
10:25-11:00	Coffee Break
11:00-11:30	Industrial Presentation by a member company – 3: The role of applied thermo in Problem Solving Excellence (PSE) in industry (<i>Antoon J.B. ten Kate, Nouryon</i>)
11:30-11:55	Overview of activities in Process Systems Engineering (PSE) at PROSYS (<i>Gurkan Sin</i>)
11:55-12:00	CERE Discussion Meeting – Closing remarks (<i>Georgios M. Kontogeorgis</i>)
12:00-13:00	Lunch (both centers/consortia)
13:30	Departure by Bus to DTU Chemical Engineering (optional)
14:15-17:00	Individual Meetings at DTU
13:00-15:00	Possibility to attend the following joint KT-Consortium & CERE program
13:00-15:00	Properties and Thermodynamics – Computer-Aided (Process and Product) Design <i>Chair: Xiaodong Liang</i>
13:00-13:15	Overview of Properties – Thermodynamic modeling at CERE/KT-Consortium (<i>Georgios M. Kontogeorgis</i>)
13:15-13:35	Computer-aided design of ionic liquids as solvents for hybrid process schemes (<i>Yuqiu Chen</i>)
13:35-14:00	Polymer Thermodynamics (<i>Nicolas von Solms</i>)
14:00-14:20	A model-based methodology for the design and selection of solvents for coating formulations (<i>Spardha V. Jhamb</i>)
14:20-14:40	Property estimation and database of pigment properties for paint design (<i>Markus Enekvist</i>)
14:40-15:00	General Discussion on Properties and Thermodynamics (<i>Georgios M. Kontogeorgis, Xiaodong Liang</i>)