DTU
Center for Energy Resources Engineering

Technical University
of Denmark

Final Program for CERE Discussion Meeting
21-23 June 2017

Hotel Comwell Borupgaard, Snekkersten, Denmark

Wednesday, 21 June

9:30-10:30 CERE Software Workshop at DTU Chemical Engineering – SPECS, GERG, Aspen User Models, Scaling, ExpertThermo *(Alay Arya, Alexander Shapiro, Xiaodong Liang, Philip Fosbøl, Kaj Thomsen)*

10:30-11:15 Lab Tour including Demonstration of the Virtual Reality Room (VR) *(Nicolas von Solms and Wei Yan)* and/or visit at DTU Chemical Engineering Pilot Plant facilities *(Nicolas von Solms and faculty from Pilot group)*

11:15 Departure by Bus from DTU Chemical Engineering to Hotel Comwell Borupgaard, Snekkersten, Denmark

12:00-13:00 **Lunch**

13:00-13:20 Welcome and News by Georgios M. Kontogeorgis

Plenary Lectures Session – 1 *(Georgios M. Kontogeorgis)* General activities and some major projects

13:20-13:40 Overview of Experimental Activities at CERE *(Nicolas von Solms)*

13:40-14:00 Demonstration of the CAPCO$_2$ software *(Philip Fosbøl)*

14:00-14:20 Overview of the COMPPLEX (2013-2017) and NextOil projects (2013-2016) (*Wei Yan)*

14:20-14:40 Overview of Geothermal projects *(Ida Lykke Fabricius)*

14:40-15:10 **A Maxwell-Stefan description of CO$_2$ permeation in PVDF *(Industrial Presentation by Jacob Sonne, NOV, Denmark)***

15:10-15:40 **Coffee Break**

Plenary Lectures Session – 2 *(Wei Yan/Ida L. Fabricius)* Projects close to completion - NextOil

15:40–16:00 Modeling of high pressure-high temperature (HPHT) fluids *(Farhad Varzandeh)*

16:00-16:20 Prediction and experimental determination of the solubility of sulfide scales at high temperatures and high pressures *(Diana Carolina Figueroa Murcia)*

16:20-16:40 Experimental study of high pressure high temperature (HPHT) fluids *(Teresa Regueira)*

16:40-17:00 Temperature effects on stiffness moduli of quartz bearing reservoir sandstone from the deep North Sea *(Tobias Orlander)*

17:00-17:20 Rock mechanical aspects of Next Oil *(Katrine Alling Andreassen)*

17:20-17:40 Coffee Break

Plenary Lectures Session – 3 *(Kaj Thomsen)* Projects close to completion – CHIGP/Compplex

17:40-18:00 Asphaltene modeling with CPA, PC-SAFT and SRK equations of state *(Alay Arya)*

18:0-18:20 A CPA-equation of state for electrolyte mixtures *(Anders Schlaikjer)*

18:20-18:40 RAND-based formulations for isothermal multihphase flash *(Duncan Paterson)*

18:40-19:00 Phase behavior in shale reservoirs with capillary pressure and adsorption effects *(Diego Sandoval)*

19:15 Dinner

Thursday, 22 June

Plenary Lectures Session – 4 *(Alexander Shapiro)* CCS and OPTION

08:15-08:35 CERE CO_2 Capture and Gas Hydrate Activities *(Nicolas von Solms)*

08:35-08:55 Overview of the OPTION project (2012-2018) *(Erling H. Stenby)*

08:55-09:35 **Trace component behavior modelling *(Industrial presentation by Miranda Mooijer, Shell, The Netherlands)***

09:35-10:00 Coffee Break

Plenary Lectures Session – 5 *(John Bagterp Jørgensen)* OPTION and more

10:00-10:20 Optimal control and production optimization *(John Bagterp Jørgensen)*

10:20-10:40 Long-range Unmanned Aerial Vehicle for High-Quality Magnetic Surveing - an Innovation Fond Denmark project: New exploration possibilities for the mineral exploration industry *(Arne Døssing Andreasen)*

10:40–11:00 How can computational fluid dynamics improve reservoir simulations and completion strategies? *(Casper Schytte Hemmingsen)*

11:00-11:45 **Reservoir Geomechanics for Field Development Planning**
(Industrial presentation by Monzurul Alam, Schlumberger, United Kingdom)

11:45-12:45 **Lunch**

Plenary Lectures Session – 6 *(Xiaodong Liang)* Theoretical Developments

12:45-13:05 On the density gradient theory in the surface tension calculations: theory, algorithms and applications (*Xiaodong Liang)*

13:05-13:25 Calculation of multiphase chemical equilibrium with non-stoichiometric methods *(Christos Tsanas)*

13:25 –13:45 Simultaneous representation of critical point and phase equilibria with equations of state (*Andre Vinhal)*

13:45-14:00 **Coffee Break**

Plenary Lectures Session – 7 *(Nicolas von Solms)* Applications

14:00–14:15 Two-phase flows in porous medium accounting for separating surface: extension onto 3D *(Alexander Shapiro)*

14:15 – 14:35 Basic sulfur corrosion mechanisms *(Henrik Lund Nielsen)*

14:35 – 14:50 CFD simulation of reservoir processes with black oil PVT description *(Igor Nesterov)*

14:50-15:10 Upscaling of enzyme enhanced CO_2 capture process *(Arne Gladis)*

15:10-15:30 Field scale recovery curve based workflow for dual porosity reservoirs *(Justin Brand)*

15:30-17:00 **Poster Session (Award for the Best Poster; Evaluation Committee: Selected members of CERE consortium and 1 external academic)**

Tobias Ritschel: Dynamic optimization of UV flash processes

Steen Hørsholt: Oil production optimization by combination of Matlab and Eclipse (E300)

Lasse Hjuler Christiansen: A least squares method for efficient and reliable short-term versus long-term optimization

Casper Schytte Hemmingsen: How can computational fluid dynamics improve reservoir simulations and completion strategies?

Xiaoyan Liu: Interactions between Kraka core plug sample and model oil in salt soultions

Yingjun Cai: Lithium battery with ionic liquid as electrolyte

Liang Mu: Hydrate thermal dissociation behavior and dissociation enthalpies in methane-carbon dioxide swapping process

Liang Mu: Phase equilibrium of DME systems with relevance to enhanced oil recovery

Arne Gladis: Evaluation of alternative desorption process without reboiler for carbonic anhydrase enhanced MDEA

Francois Kruger: Uncertainty analysis and evaluation of Cubic-Plus-Association parameterization

Susana Almeida: Gas permeation and solubility measurements and modelling for polymer pipelines in offshore applications

Christos Tsanas: Phase Equilibrium Modeling for the DME Enhanced Water-flooding

Amin Abouardini and Casper Mølby Berg: A Feasibility Study of Hydrocarbon Gas Injection in Skjold Field

Eirin Limos Abrahamsen: Experimental Investigation of Structure II Hydrate Kinetic Inhibition

Li Sun: Modeling CO_2 semi-clathrate hydrate related systems: literature review and database (from KTconsortium meeting)

Mauro Torli: The SYNFERON project (from KTconsortium meeting)

Edgar Camacho: Inhomogeneous fluid behavior: density functional theory approaches (from KTconsortium meeting)

Anders Schlaikjer: Development of CPA for electrolyte mixtures (from KTconsortium meeting)

Alay Arya: Modeling of asphaltene precipitation: A flow assurance problem (from KTconsortium meeting)
Mirhossein Taheriotaghsara: Smart Water – a wettability modifier in chalk?

Jiasheng Hao: Investigation of fluid-rock interactions for SmartWater in carbonate reservoirs

Georgios Aloupis: A fair comparison of CPA and PC-SAFT on modeling gas hydrate-related systems

Niklas Bennedsen: Evaluation of theories for the prediction of interfacial tension and contact angles in polymer-related solid surfaces

Kasper Dupont Enemark: Permeability in deep North Sea sandstones as predicted from NMR

Ioannis Tsivintzelis and Costas Panayiotou: On the dimerization of carboxylic acids: An equation of state approach
Jesper Poulsen and Frederik Topsøe: Exclusion Zone close to Nafion surfaces – proof in CERE laboratories

Adem Rosenkvist Nielsen Aouichaoui, Maria E. Mondejar, Stefano Cignitti and Fredrik Haglind: Modelling of a generalized BWR equation of state for halogenated olefins of relevance to Organic Rankine Cycle systems

Artem Alexeev: Mathematical Models for Advanced Waterflooding: Oil Ganglia and Surface Chemistry of Carbonate rocks

Karen Gulbæk Schmidt: Trends in the field of petrophysics

Ivanka Orozova-Bekkevold: Forward geomechanical modelling in exploration and production

Nomiki Kottaki: HPHT PVT study of a volatile oil up to 473 K

Maria-Lito Glykioti: Density and compressibility measurements of reservoir fluids at high pressures and high temperatures

Yiqun Liu: High pressure phase behavior of asymmetric mixtures for oil production

Eirin Karakatsani: Modeling sulfur distribution in the Claus process

Xiaodong Liang: A fair comparison of CPA and PC-SAFT on modeling gas hydrate-related systems

Tianyuan Wang: Modeling of CO_2-MDEA-water systems using the CPA equation of state with a simplified approach

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17:00-18:30 **Member Round Table in Plenum**

- This year's Discussion Meeting so far and what's next
- Evaluation of the 2017 Discussion Meeting – suggestions for changes
- Questionnaire for CERE member companies
- New industrial collaborations – future perspectives – next year's Discussion Meeting
- Priority topics and new developments (short/medium term)
- Long term perspectives and future plans

19:00 **Aperitif**

19:30 **Conference Dinner**

After Dinner Talk by Dr. Nikolaj Sorgenfrei Blom
"Can Water Structure Research Become a New Innovation Driver ?"

Friday, 23 June

Plenary Lectures Session – 8: *(Philip L. Fosbøl)* New Directions I

08:30-08:45 20 years with CPA: What's easy, what's not, what's next *(Georgios M. Kontogeorgis)*

08:45-09:15 **Computational fluid dynamics simulations of flow in oil wells *(Invited academic talk by Jens Honore Walther, DTU-Fluid Mechanics, Denmark)***

09:15-09:30 Thermodynamics, design, simulation and benchmarking of biofuel processes *(Mauro Torli)*

09:30-09:45 Inhomogeneous fluid behavior: density functional theory approaches *(Edgar Camacho)*

09:45-10:05 Thermodynamic and process challenges in subsea gas processing *(Francois Kruger)*

10:05 –10:35 **Coffee Break**

Plenary Lectures Session – 9: *(Georgios M. Kontogeorgis)* New Directions II

10:35-10:50 Effect of Fines Particle Size on Emulsion Formation *(Muhammad Waseem Arshad)*

10:50-11:10 Controls on chalk stiffness in the Danish Central Graben *(Leonardo Teixeira Pinto Meireles)*

11:10-11:25 Modeling CO_2 semi-clathrate hydrate related systems – Phase I: fluid phase equilibria *(Li Sun)*

11:25-11:40 Feasibility of geothermal energy extraction from medium depth Danish limestone aquifers *(Laura Paci)*

11:40-12:00 Future Perspectives and Closing Remarks *(Georgios M. Kontogeorgis)*

12:00-13:00 **Lunch**

13:30 Departure by Bus to DTU Chemical Engineering

14:15-17:00 Individual Meetings