

KT Consortium Annual Meeting 2018

19-21 June 2018

Rungstedgaard
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Preliminary Technical Program

Tuesday 19 June 2018	
Morning-Noon	Arrival to the hotel & registration (after 11:00 a.m.)
12:00-13:00	Lunch (jointly with CERE)
13:00-16:00	ICAS and CERE Software Workshop Assistant Professor Xiaodong Liang, Post Doc Alay Arya and PhD Students Nipun Garg and Spardha V. Jhamb
13:00 - 13:10	Introduction and overview of ICAS (Xiaodong)
13:10 - 13:30	Pure component properties and models: Database Manager and ProPred (Alay)
13:30 - 13:55	ProCAMD (Computer Aided Molecular Design) / VPPD Lab (Spardha/Alay)
13:55 - 14:20	SolventPro (Solvent Selection and Design Framework) (Xiaodong)
14:20 - 14:50	Coffee break
14:50 - 15:20	Super-O: Superstructure Optimization & SustainPro, LCSOft (Nipun)
15:20 - 15:50	Selected CERE software (Alay & Xiaodong) - Electrolyte CPA (MATLAB), ThermoSystem, DGT for interfacial tension - and if time permits it Scale-CERE (Kaj Thomsen) Alternatively there will be possibility to attend one of the other two parallel sessions in CERE Discussion Meeting (either parallel session 5: SYNFERON project , or parallel session 6: DHRTC collaborations , more information will follow via the CERE Discussion Meeting Program)
16:00-18:30	Joint CERE & KT Consortium Poster Session
19:00	Welcoming drink
19:30-22:00	CERE & KT Consortium Galla Dinner Best Poster Awards (CERE & KT Consortium) – with separate award ceremony

Wednesday 20 June 2018 (Technical Program 08:40-15.30)**Common morning program for CERE & KT Consortium**

Chair: Professor Georgios M. Kontogeorgis

08:40-08:50	CERE & KT-Consortium: Two centers, two consortia but much in common (Professor 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)
	The John x 3 Session
09:20-09:40	Thermodynamics, simulation, control, optimization, and scientific computing (Associate Professor John Bagterp Jørgensen)
09:40-10:00	The need for property prediction and thermodynamic data for biological conversions (Professor 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	Invited lecture by CERE member company BP, Dr. Nikos Diamantonis: Physical properties in different stages of process development
11:30-12:00	CERE Discussion Meeting – Closing remarks (Professor Georgios Kontogeorgis)
12:00-13:00	Lunch (all/both Consortia)
13:00-15:00	Joint KT Consortium & CERE program (optional for CERE)
13:00-13:30	Invited lecture by Dr. Ioannis Tsvintzelis: Phase Equilibria for biodiesel-related compounds with CPA
13:30-13:50	Phase equilibria modelling applied to design and analysis of a lipids related process (PhD student Olivia Ana Perederic)
13:50-14:20	On the PT Flash calculations (Assistant Professor Xiaodong Liang)
14:20-14:40	A General Methodology for Chemical Substitution (PhD student Spardha V. Jhamb)
14:40-15:00	Inherently safer design of chemical processes (PhD student Saeed Eini)
>15:30	Departure of CERE consortium members and CERE co-workers – after that program only for KT Consortium
16:00-18:00	Social program to the Karen Blixen Museum
18:00-20:30	KT-Consortium Dinner // After Dinner Talk
20:30-21:30	KT Consortium Advisory Board Meeting

Thursday 21 June 2018 (Technical Program 8:30-14:45)**Presentations by PhD students and Post Docs**

Chair: Professor John Woodley

08:30-08.50	Energy Efficient Design of Ionic Liquid based Gas Separation Processes (PhD student Xinyan Liu)
08.50-09.10	Simulation and evaluation of utilization pathways of biomasses based on thermodynamic data prediction (Researcher Hongliang Qian)
09.10-09.30	Integrated Solvent-Membrane and Process Design Method for Hybrid 2. Reaction-Separation Schemes (PhD student Yuqiu Chen)
09.30-09.50	Sustainable and Innovative Chemical and Biochemical Solutions through an Integrated Systematic Framework (PhD student Nipun Garg)
10:00-10.30	Coffee Break - Demonstrations and Networking
	Invited Session
10:30-11.00	Invited 1: Industry – 1: Schneider Electric, US, Nevin Gerek: Challenges and solutions for next generation process simulators
11:00-11.30	Invited 2: Dr. Ioannis Tsivintzelis: Pharmaceuticals and polymers phase equilibria
11:30-12.00	Invited 3: Associate Professor Kaj Thomsen: Extended UNIQUAC - a successful model for electrolyte applications
12.00-12.30	Current Status and Challenges in Electrolyte Thermodynamics (Professor Georgios Kontogeorgis)
12.30-13.30	Lunch
13:30-14.00	Invited-4: Industry – 2: Syngenta Ltd., UK, Patrick Piccione: More Industrial Reflections on Modelling of Fine Chemicals and Seeds Process/Product Design
14.00-14.45	Conclusion of KT-Consortium Annual Meeting (Professor Georgios Kontogeorgis) <ul style="list-style-type: none">- Oral Awards for KT-Consortium PhD students and Post-Docs.- Open Discussion with all, conclusion of the meeting and future plans.- What worked well with this year's Annual Meeting and what should we change next time?- What else/more can DTU Chemical Engineering contribute to KT Consortium?
14:45	End of meeting – bus transportation to DTU, bld. 229
15:15	Arrival at DTU, bld. 229
15:30-16:30	PILOT PLANT tour, bld. 228 (if of interest)

KT Consortium - Poster Presentations 2018

No.	Personnel	Poster Title
	MSc/BSc Students:	
P1	MSc Martin Due Olsen	Thermodynamic modeling of the solubility of pharmaceuticals with the PC-SAFT EOS
P2	BSc Kasper Kofod Boss	Cross-association combining rules in the PC-SAFT EOS
	PhD Students:	
P3	Xinyan Liu	Property Modeling of Ionic Liquids for Gas Separation Processes
P4	Spardha V. Jhamb	Substitution from Chemical-based Products
P5	Yuqiu Chen	Integrated Ionic Liquid and Process Design involving Hybrid Separation Schemes
P6	Olivia Ana Perederic	Systematic methods and tools for lipids process technology
P7	Nipun Garg	A multi scale and multi-level computer aided approach for Process Intensification
P8	Saeed Eini	Multi-objective optimization of an LNG process
	Researchers:	
P9	Alay Arya	Recent application of CPA for flow assurance (asphaltenes)
P10	Hongliang Qian	Exergy efficiency based design and analysis of utilization pathways of biomasses