

KT Consortium Annual Meeting 2019

12-14 June 2019

Beach Hotel Marienlyst

Preliminary Technical Program

Wednesday 12 June 2019	
Morning-Noon	Arrival to the hotel & registration (after 11:00 a.m.)
12:00-13:00	Lunch (jointly with CERE)
13:00-15:00	ICAS Software Workshop Assistant Professor Xiaodong Liang, Software Manager and PhD Students Nipun Garg, Spardha V. Jhamb and Markus Enekvist
13:00-13:10	Introduction and overview of ICAS (Xiaodong)
13:10-13:25	Pure component properties and models: Database Manager and ProPred (Software Manager)
13:25-13:40	ProCAMD (Computer Aided Molecular Design) / VPPD Lab (Spardha and Markus)
13:40-14:00	SolventPro (Solvent Selection and Design Framework) (Xiaodong)
14:00-14:25	Development of a Virtual Educational BioProcess (Simoneta Cano de las Heras)
14:25-14:45	Super-O: Superstructure Optimization & SustainPro, LCSoft (Nipun)
14:45-15:00	Azeopro (Software Manager)
	Alternatively there will be possibility to attend one of the other two parallel sessions in CERE Discussion Meeting (either parallel session on SYNFERON project , or parallel session on DHRTC collaborations , more information will follow via the CERE Discussion Meeting Program)
15.00–16.00	Short video presentations of posters (in plenum)
16:00-18:30	Joint CERE & KT Consortium Poster Session
19:00	Welcome drink
19:30-22:00	CERE & KT Consortium Gala Dinner Best Poster Awards (CERE & KT Consortium) – with separate award ceremony

Thursday 13 June 2019 (Technical Program 08:40-15.30)	
Common morning program for CERE & KT Consortium	
Chair: Professor Georgios M. Kontogeorgis	
08:40-08:45	CERE & KT-Consortium: Welcome, Introduction to the two consortia and common program of the day (Georgios M. Kontogeorgis)
08:45-09:00	Software in CERE and Software in KT Consortium (ICAS) – A short introduction (Software Manager, Xiaodong Liang)
09:00-09:15	Experimental activities in CERE (Nicolas von Solms)
09:15-09:50	Industrial Presentation by a member company – 1 (DSM)
09:50-10:25	Industrial Presentation by a member company – 2 (Mitsubishi)
10:25-11:00	Coffee break
11:00-11:30	Industrial Presentation by a member company – 3 (Nouryon)
11:30-11:55	Overview of activities in Process Systems Engineering (Gürkan Sin)
11:55-12:00	CERE Discussion Meeting – Closing remarks (Georgios M. Kontogeorgis)
12:00-13:00	Lunch (all/both Consortia)
13:00-15:00	Joint KT Consortium & CERE program (optional for CERE) Properties and Thermodynamics Computer-Aided (Process and Product) Design (Chair: Xiaodong Liang)
13:00-13:15	Overview of Properties – Thermodynamic modeling in CERE/KT-Consortium (Professor Georgios M. Kontogeorgis)
13:15-13:35	Computer-aided design of ionic liquids as solvents for hybrid process schemes (PhD student Yuqiu Chen)
13:35-14:00	Polymer Thermodynamics (Associate Professor Nicolas von Solms)
14:20-14:40	A Model-based methodology for the design and selection of solvents for coatings formulation (PhD student Spardha V. Jhamb)
14:40-15:00	Property estimation and database of pigment properties for paint design (PhD student Markus Enekvist)
15:00-15:30	General Discussion on Properties and Thermodynamics (Coordinators: Georgios M. Kontogeorgis, Xiaodong Liang)
>15:30	Departure of CERE consortium members and CERE co-workers – after that program only for KT Consortium
17:00-18:00	Social program (Louisiana Museum of Modern Art)
18:00-20:30	KT-Consortium Dinner
20:30-21:30	KT Consortium Advisory Board Meeting

Friday 14 June 2019 (Technical Program 8:30-14:45)	
Process Design and Simulation	
Chairs: Professor John Woodley, Associate Professor Gürkan Sin	
08:30-08:50	Ionic liquid design and process simulation for shale gas separation (PhD student Xinyan Liu)
08:50-09:10	A generic phenomena-based synthesis method for process intensification (PhD student Nipun Garg)
09:10-09:30	Application of deep learning for process modeling and monitoring (Post Doc Soonho Hwangbo)
09:30-09:50	Downstream processing of biochemical processes (PhD student Kristian Meyer)
09:50-10:10	A Modular and Libre Modeling Environment for Computer-Aided Process Design and Optimization (PhD student Mark Jones)
10:10-10:40	Coffee Break
10:40-11:05	Cyclic separations: Theory, modeling, simulation and experiments (Associate Professor Jens Abildskov)
11:05-11:30	Analyzing Plant-wide Operation Challenges in Biochemical Downstream Production Plants (Associate Professor Jakob K. Huusom)
11:05-11:50	Large Scale Pharmaceutical Crystallization Process Modeling (PhD student Merve Öner)
11:50-12:10	Towards development of a decision support tool for conceptual design of wastewater treatment plants using stochastic simulation optimization (PhD student Resul Al)
12:10-12:30	Novel strategies for control and modelling of bio-processes using advanced image analysis (PhD student Rasmus F. Nielsen)
12.30-12.45	General Discussion on Process Design and Simulation (Coordinators: Professor John M. Woodley and Associate Professor Gürkan Sin)
12.45-12.55	Conclusion of KT-Consortium Annual Meeting (Professor Georgios M. Kontogeorgis)
13:00-14:00	Lunch (+ oral award)
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)

Preliminary List of posters

Xinyan Liu

Ionic liquid screening for shale gas separation

Spardha Jhamb

Solvent selection for coating formulation: method, applications and issues

Yuqiu Chen

Ionic liquid design and process simulation for separation of aqueous solutions

Nipun Garg

Phenomena based synthesis-intensification: generalized method and case studies

Markus Enekvist

Property estimation and database of pigment properties for paint design

Ergys Pahija

Sequential Monte Carlo to monitor Lactic Acid Bacteria Fermentation

Edgar Vergara

Modelling of Asphaltene Adsorption with Advanced Molecular Models: A Classical DFT Approach

Li Sun

Application of Electrolyte CPA Equation of State in Modeling of Absorption Refrigeration Cycle

Jiahuan Tong

Molecular simulation of high concentration lithium-containing electrolyte solutions

Xianglei Meng

Ionic liquids as benign solvents for CO₂ utilization reactions

Enrico Mancini

Development novel systematic strategic for downstream process design

Mauro Torli

The SYNFERON project – the conclusion

Nikolaus Vollmer

Process Design, Optimization and Supply Chain Analysis for Biotechnological Production of Xylitol