Imperial College London

Centre for Process Systems Engineering
2016 Seminar Series: The Next Generation

UCL

The next generation of methods and tools for Computer-Aided Molecular Design

Prof. André Bardow
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Abstract:

What is the optimal molecule? Answer: It depends – on the specific application. Thus, the specific application should guide the design of novel molecules. We therefore present methods to integrate computer-aided molecular design (CAMD) directly into process design for a specific application. The resulting process design optimization simultaneously considers process settings and molecular degrees of freedom. Due to the practically unlimited molecular design space, efficient strategies are required to solve the simultaneous design problem. Here, we present the Continuous-Molecular Targeting (CoMT-CAMD) framework developed in cooperation with Prof. Joachim Gross (Stuttgart) over the last years. The key feature enabling the efficient solution of the simultaneous design problem is a physically-based thermodynamic model. Modern thermodynamic models provide a rich molecular picture which can be exploited in CAMD for both more efficient solution methods and for more accurate molecular designs. The benefit of modern thermodynamic models in CAMD will be demonstrated using both the PC-SAFT Equation-of-State and COSMO-RS. Case studies from the design of solvents for liquid-liquid extraction and of working fluids for Organic Rankine Cycles illustrate the potential of simultaneous process and molecular design based on modern thermodynamic models.

Bio:

André Bardow is full professor and institute head at the Chair of Technical Thermodynamics at RWTH Aachen University, Germany. After studying mechanical engineering with a major of chemical engineering at RWTH Aachen University, and Carnegie Mellon University, Pittsburgh, PA, he received a Ph.D. in process systems engineering supervised by Prof. Wolfgang Marquardt at RWTH. He was a Postdoc at ETH Zurich, Switzerland, before becoming assistant and later associate professor in the Department of Process & Energy at TU Delft, The Netherlands. In 2010, he returned to RWTH. For the last 6 months, he has been a visiting professor at the Bren School for Environmental Science & Management at the University of California, Santa Barbara. The scope of his work spans across all scales of thermodynamics from molecules to the plant level. His research aims at integrating life-cycle thinking into engineering design for sustainable energy and chemical industries.

4 May 2016, 4PM
CPSE Seminar room, RODH C615

C O G
computational optimisation group

CPSE Seminar room, RODH C615, Roderic Hill Bldg, Chemical Engineering department, Imperial College London, London SW7 2AZ
This event is free and open to the public. No registration is required.
Reception drinks after the seminar in CPSE Common room (top floor Roderic Hill Bldg).

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