

## **“Model-Based Chemical Product Design and Analysis”**

**Wednesday  
April 1, 2020  
3:00 pm  
Wu and Chen Auditorium  
Levine Hall**



**Rafiqul Gani**  
Distinguished Visiting Professor  
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### **Abstract**

Chemical products are usually designed and developed through heuristic rule-based and/or trial-and-error experiment-based approaches. Although this kind of approaches often lead to safe and reliable product designs, since it is not practically feasible to consider all alternatives, it may not be possible to find the optimal product. As an alternative approach, the use of model-based design methods has been gaining increased attention as they have the potential to rapidly generate and/or screen product candidates in a much larger design space, and therefore reduce cost for chemical product design and development. If needed data and/or models giving reliable estimations for product properties and functions are available, model-based chemical product design methods may be applied for design and analysis of many chemical products classified as single species (such as refrigerants, solvents, and chemical substitutes) and multiple species (such as fuel blends, insect repellents, detergents and paint formulations). The seminar will highlight, with special emphasis on predictive chemical product property modelling, a model-based computer-aided framework plus associated methods and software tools for systematic design and analysis of a wide range of chemical products.

### **Bio**

Rafiqul Gani, Ph.D. is currently a distinguished visiting professor at Zhejiang University, at Tsinghua University and at Texas A&M University. For 34 years, Prof. Gani worked at the Department of Chemical & Biochemical Engineering, Technical University of Denmark, and is the former head and co-founder of CAPEC. Prof. Gani served as an editor-in-chief of the Computers and Chemical Engineering journal and currently serves on the editorial advisory boards of several journals. Prof. Gani has been awarded Doctor Honoris Causa degrees from the Politehnica University of Bucharest, University of Pannonia, and Babes-Bolyai University. Prof. Gani is the ex-president of the EFCE, a member of the Danish Academy of Science, a Fellow of the AIChE, and a Fellow of IChemE. He received the AIChE Computers in Chemical Engineering award in 2015 and the EFCE Jacques Villiermaux Medal in 2019. In 2018, Prof. Gani co-founded the PSE for SPEED Company. His current research interests continue with the development and application of computer aided methods and tools for modelling; property estimation; process-product synthesis, design and intensification; and process-tools integration with emphasis on energy, sustainability and application of a systems approach.

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