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PSE for SPEED
Sustainable Product-Process Engineering, Evaluation & Design

Time for a new class of methods and computer aided tools to address the challenges facing us?

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The need for innovative and significantly better solutions than we currently can obtain has become critical and urgent because of the grand challenges of health, food, water, energy and environment that we are facing. The way we convert our resources to the chemicals-based products that we need for the survival of our society is clearly not working as evidenced by the sharp drop of earth's biocapacity, measured in terms of hectares per person. The solution of this complex problem offers the opportunity for fundamental advances in science and technology. However, one area that needs urgent attention is our solution approach where we predominantly either use experiment-based trial and error approaches, or model-based computer aided techniques. While the former guarantees an experimentally verified solution but does not guarantee that better solutions do not exist, the later is able to quickly find the best solution within a defined search space using validated models. Both, however, lack predictive capabilities. That is, ability to find solutions beyond the scope of the technologies they are employing. This presentation focuses on issues related to model-based computer aided techniques and what must be done to overcome them.

The development and use of the so-called process simulator has without doubt achieved great success. The petroleum and related industries have made significant progress towards achieving reliable design, safer operation, with for example, lower energy consumption and higher profit. This success, however, has lead to a negative trend, that is, replaced the trial and error experiment-based solution approach to the trial and error simulator-based solution approach, which is a faster and less expensive option. However, does it lead to the innovative and significantly better solution that we now need? The current unit-operation based process simulators have an inherent deficiency that they do not have the capability to find new and innovative processing routes involving newly developed technologies. That is, should we look for solution approaches that are not so simulator specific? Are simulators able to solve the current problems we are interested in? If not, should we develop new methods & tools, or, should we wait until the simulators have the needed capabilities, such as the ability to find innovative solutions? A critical issue here is to understand the role of the process simulator – it is by definition, a tool to verify and not to determine the synthesis of a processing route, the actual process design, or the operation design or sustainable process alternatives and many more. They should be used for the purpose they are developed for.

Clearly, a new class of methods and associated model-based computer aided tools are needed, where predictive and innovative capabilities are provided. Also, the many current and future needs, which may change, must be satisfied. For example, capabilities to synthesize new processing routes; to design chemicals-based products; to integrate resource management-utilization; to synthesize new intensified operations; to generate sustainable process alternatives and many more. Therefore, rather than provide large, complex and rigid process simulators, it could be useful to provide tailor-made problem specific tools configured from a library of different software components (databases, models, design work-flows, analysis tools, solvers, etc.) according to the needs of the user. Note that here, the process simulator is one of many components and the models in the component library need to have predictive capabilities. It should be possible to generate tailor-made tools of different scales with smooth transition from one scale to the other for similar applications.

Dr. Rafiqul Gani retired at the end of 2017 as professor of systems design at the Department of Chemical & Biochemical Engineering, The Technical University of Denmark and the former head and co-founder of the Computer Aided Process Engineering Center (CAPEC). He has published 491 peer-reviewed journals-proceedings articles plus book chapters and delivered over 350 lectures, seminars and plenary/keynote lectures at international conferences, institutions and companies all over the world. Professor Gani is the former editor-in-chief of the Computers and Chemical Engineering journal (2009-2015), editor for the Elsevier CACE book series and currently serves in the editorial advisory boards of the following journals: Computers and Chemical Engineering, Sustainable Production & Consumption, Processes and BMC Chemical Engineering. Professor Gani has been awarded three Doctor Honoris Causa degrees from University Politehnica Bucharest, University of Pannonia and Babes-Bolyai University. Professor Gani is the ex-president of the EFCE (European Federation of Chemical Engineering, finishing his 2nd term at the end of 2017); a member of the Danish Academy of Science; a Fellow of the AIChE and a Fellow of IChemE. He was awarded the AIChE (CAST Division) Computers in Chemical Engineering 2015 award in November 2015. Dr. Gani is the co-founder and CEO of the company "PSE for SPEED" providing innovative, accurate and consistent engineering solutions very fast to industrial clients. He is also a Distinguished (visiting) Professor at Zhejiang University (Hangzhou, China) and at Tsinghua University (Beijing, China) and a Visiting Professor at Texas A&M University, College Station (USA(. 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 process-tools integration with emphasis on energy, sustainability and application of a systems approach

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