

PSE2015 and ESCAPE25 Plenary Lecture:

Multi-Level Design of Process Systems for Efficient Chemicals Production and Energy Conversion

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In the past decades significant progress in increasing the productivity, selectivity and sustainability of chemical production and energy conversion processes has been made. Nevertheless, in order to cope with the challenges of the future, breakthroughs in process systems engineering are necessary in order to find “dream processes” for synthesizing chemicals and transforming energy, to enable the transition from fossil fuels and petrochemical feed stocks to renewable materials and energy, to close carbon dioxide cycles, to enhance efficiency significantly, and to incorporate new functionality in materials and products.

For this purpose, new scientifically founded systems engineering approaches need to be developed, able to deal with the inherent multi-level structure of any production system. Very efficient process systems might be designable if engineers succeed to consider all essential levels involved in the process system hierarchy, namely the molecular level, phase level, process unit level and plant level [1]. But any multi-level design strategy will be successful only if mathematical process models, computer experiments and wet-lab experimental data are closely combined. Thereby, advanced quantitative understanding of complex process systems can be attained which will open new paths for translating scientific results into practical solutions.

In the present contribution, a model-based methodology is presented which derives process design decisions at different levels of the process hierarchy under consideration of various process intensification options. This approach integrates optimal experimental design, process synthesis and process analysis. The proposed methodology is demonstrated for selected challenging process design tasks, e.g. Diels-Alder synthesis in organic solvents [2], alkene hydroformylation using homogeneous Rhodium catalysts [3], shape-selective crystallization of particles [4], and on-board hydrogen production for fuel cell vehicles [5].

References

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