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A systems engineering approach to managing the complexity in sustainable chemical product-process design

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Abstract

Chemical product-process design consists of finding the identity of the candidate chemical product, designing the process that can sustainably manufacture it and verifying the performance of the product during application. The chemical product tree is potentially very large; starting from a set of basic raw materials, to a bigger set of basic chemical products, to an even bigger set of intermediates, and finally, to a very large number of refined chemicals and consumer products. At the top, the chemical products are usually from the life sciences, pharmaceutical, food and related industries while at the lower-middle levels, the chemical products are usually from the oil, petrochemical and chemical industries. These lower-middle level chemicals are usually produced in large amounts and the use of model (knowledge) based tools in the design/analysis of their processes are quite common. Problems associated with sustainable product-process design, however, involve several additional features, such as, *Multi-scale; Multidiscipline; & Multi-tools* that make these problems large, complex and difficult to solve efficiently and reliably. That is, for sustainable product-process design, it is necessary to manage complex situations requiring the handling of data and knowledge from different sources and at different scales of time and size (from micro to mega). Use of a systems approach that can efficiently *manage this complexity* therefore becomes desirable. An integrated computer aided system (ICAS) has been developed to efficiently manage the complexity for sustainable chemical product-process design. ICAS consists of a collection of state of the art methods and tools such as knowledge (data, model, equipments, operations) libraries; templates and work-flows for synthesis/design; and, efficient numerical solvers. Problems such as design of energy efficient and sustainable intensified processes, design of environmentally friendly solvents, retrofit design of chemical processes for improved sustainability and many more can be solved and analyzed efficiently and reliably through ICAS.