243u Structured Phenomena-Based Modelling of Chemical Processes: a Pse Point of View to Support Innovative Process Design

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Some step-change design philosophies are currently emerging in response to the requirements for sustainable processes. Process Intensification (including multifunctional processes) is representative of current innovative design philosophies. The basis for its success is to take apart the paradigm of Unit Operations. Generation and evaluation of novel designs require the fundamental analysis and understanding of process phenomena without the spatial constraints of conventional unit operation models. Optimal processes are found when they are designed to perform at the right timescale and lengthscale, involving a multilevel design and multiscale modeling.

This contribution explores, unifies and adapts the phenomena-based concepts built upon the General Systems Theory and uses them to approach innovative design of chemical processes. The process design is refined in various levels by means of more fundamental and flexible building blocks structured by the process tasks, the phases involved and the phenomena taking place within them. The generation of multilevel models representing these building blocks can be supported by computer-aided tools built in object-oriented architectures. Some academic prototypes have been developed with a phenomena-based structure to aid in the complex process of modelling. However, their availability is limited and not well disseminated. We demonstrate how these phenomena-based structuring concepts can be used consistently with the available commercial object-oriented and equation-based tools for immediate computer implementation of the theoretical framework.

The proposed approach provides both insight into the processes being modelled and an appreciation of the cause and effect. These concepts should support innovative process design by enabling generation and evaluation of alternatives to encourage a faster implementation of PI design concepts and ultimately devices.