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Achieving Process Intensification: A Phenomena-Based Synthesis/Design Methodology

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In recent years, Process Intensification (PI) has attracted considerable interest as a potential means of process improvements and to meet the increasing demands for sustainable production [1]. PI seeks to improve processes by increasing efficiency, reducing energy consumption, operational costs, volume and waste as well as simplifying the flowsheet. Thus, a variety of intensified operations and equipment have been developed by academia and industry but, to date, only a limited number of intensified technologies have achieved implementation, such as reactive distillation, dividing wall columns and reverse flow reactors [2]. One major reason for this is that the identification of the best PI option with the currently used techniques is neither simple nor systematic.

In previous work [3] we reported the development of a general computer-aided systematic synthesis/ design methodology. In order to manage the complexity of the potentially large number of intensified options, the optimization problem is solved by a decomposition approach. In this methodology, redundant intensified options were systematically removed by checking against predefined constraints. However, at present, this methodology is limited to already pre-defined PI unit operations which can be retrieved, together with all the necessary information for synthesis and design of each, from a knowledge base tool. In order to *invent* new unit operations and based on them, new process designs and flowsheets, it is necessary to investigate PI options at the phenomenological level [4, 5], which is the topic of this contribution. The basis of the phenomena-based process synthesis is phenomena building blocks consisting of mass, component, energy and momentum balances as well as connectivity rules between the phenomena building blocks. Two different connections between phenomena exist: A connection implying the simultaneous occurrence of phenomena or a connection implying the sequential occurrence of phenomena which depends on the operational window of the phenomena involved. Based on this approach, a general methodology has been developed for phenomena-based synthesis/design, similar to the one for pre-defined PI unit operations [3]. First, the process design problem is defined, in terms of a set of product qualities and quantities as well as additional process constraints and the desired (target) process improvement. Next, this information is analyzed to identify all potential phenomena building blocks and their corresponding operational windows. Based on this, the phenomena building blocks are joined together according to connectivity rules to match the defined process intensification targets and a superstructure of flowsheet options is generated. In the following step, the generated options are screened in terms of additional logical and structural constraints as well as performance specifications before unit operations are identified. For example, a sequence of at least three simultaneous ideal mixing and reaction phenomena can be identified as a plug flow reactor. In the penultimate step, a reduced optimization (NLP) problem is solved to identify the best intensified flowsheet. The advantage of the phenomena-based process synthesis and design is that it generates potentially *novel* process options because the initial search space is wider and allows space beyond those involving existing unit operations and is truly predictive. Also, the method provides simultaneous development of the necessary process models.

In this contribution the application of the phenomena-based process synthesis/design methodology implemented within a computer-aided framework will be presented together with a selected example of industrial importance.

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[3]   Lutze, P., Gani, R., Woodley, J.M. Process Intensification: A perspective on process synthesis. Chem Eng Process 2010;

49, 6, 547-558.

[4]   Freund, H., Sundmacher, K. Towards a methodology for the systematic analysis and design of efficient chemical processes: Part 1. From unit operations to elementary process functions. Chem Eng Process 2008; 47, 12, 2051-2060.

[5]   Papalexandri, K.P., Pistikopoulos, E.N. Generalized modular representation framework for processs synthesis. AIChE J 1996; 42, 4, 1010-1032.

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