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Sustainable process synthesis–intensification

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ABSTRACT

Chemical industry is facing global challenges such as the need to find sustainable production processes. Process intensification as part of process synthesis has the potential to find truly innovative and more sustainable solutions. In this paper, a computer-aided, multi-level, multi-scale framework for synthesis, design and intensification of processes, for identifying more sustainable alternatives is presented. Within the framework, a three stage work-flow has been implemented where, in the first "synthesis" stage an optimal processing route is synthesized through a network superstructure optimization approach and related synthesis tools. In the second, "design" stage, the processing route from the first stage is further developed and a base case design is established and analyzed. In the third, "innovation" stage, more sustainable innovative solutions are determined. The application of the framework is illustrated through a case study related to the production of di-methyl carbonate, which is an important bulk chemical due to its multiplicity of uses.

1. Introduction

In the chemical industry improvements related to the use of sustainable technologies and efficient use of resources are needed in order to achieve reductions in energy consumption, waste generation, environmental impact and cost. Process improvements are typically achieved through an evolutionary approach, where knowledge gained from process understanding together with expert knowledge on process engineering is applied. The limitation with this approach, however, is that new, innovative and more sustainable process designs may not be found because the search space employed is limited in size in the trial and error, experiment-based approaches. The same is true for model-based solution approaches where the models employed have limited application range.

The objective of process synthesis should be to find the best processing route, from among numerous alternatives, to convert given raw materials to specific (desired) products, subject to predefined performance criteria. Hence, process synthesis involves analysis of the problem to be solved, and, generation, evaluation and screening of process alternatives so that the best process option can be identified. Process synthesis is usually performed through the following three classes of methods: (1) Rule based heuristic methods, which are defined from process insights and know-how; (2) Mathematical programming based methods, where the best flowsheet alternative is determined from network superstructure optimization. This class of method is useful when the system is well defined and many combination of alternatives are to be considered; (3) Hybrid methods that uses process insights, know-how, rules and mathematical programming. That is, models are used to obtain good physical insights that aid in reducing the search space of alternatives so that the synthesis problem to be solved will involve less alternatives.

Process intensification (PI) has been defined as the improvement of a process through the targeted enhancement of performance-limiting phenomena (Lutze et al., 2013) at different scales. At the plant/process scale the entire process is considered. At the unit operations scale the individual unit operations that comprise the process are considered. At the task scale the functions performed by the unit operations are considered. A task is defined as the function performed by a unit operation, for example, a flash vessel or a distillation column represent separation tasks. At the phase/phenomena scale the phenomena building blocks (see Section 2.3.1) that satisfy and thereby, make a task feasible are considered, while, at the molecular scale (Freund, Sundmacher, Ullman, Lutze et al., 2010) which is mainly considered for reactive systems, the molecular behavior of the molecules that affect the phenomena are

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considered. According to Van Gerven and Stankiewicz (2009), this enhancement can be achieved within four domains: process structure, energy, synergy and time. One example of PI at the process/plant level is a hybrid distillation scheme which is an external integration of two or more different unit operations that include at least one operation, that is, a conventional distillation column, in order to satisfy a separation task (Babi and Gani, 2014). Here, the integration of membrane separations with distillation to overcome thermodynamic boundaries such as azeotropes (Lutze and Gorak, 2013) could be considered. Divided wall columns are examples of PI at the unit operation, task or functional scales (Asprion and Kaibel, 2010; Halvorsen and Skogestad, 2011; Madenoor Ramapriya et al., 2014) while, membrane reactors (Assabumrungrat et al., 2003; Van Baelen et al., 2005; Inoue et al., 2007) or reactive distillation columns (Agreda et al., 1990; Shah et al., 2013; Holtbruegge et al., 2014) are examples of PI that improve the conversion in a reaction through the in situ removal of a product.

Similar to process synthesis, in principle, PI could also be performed using the same three classes of methods. However, rule-based heuristic methods and the mathematical programing based methods have not been developed for the intensification of entire processes. For the design of specific hybrid/intensified unit operations within a process several methods (Bessling et al., 1997; Amte, 2011; Caballero and Grossmann, 2004) have been reported. For hybrid methods, a scheme for systematically achieving process intensification has been proposed by Lutze et al. (2013). Also, other hybrid schemes have been developed for intensifying specific parts of a process, for example, at the phenomena and molecular level (Peschel et al., 2012; Rong et al., 2008). Therefore, since process intensification aims at increasing the efficiency of processes, performing process synthesis and intensification together, should lead to improved and more sustainable process deigns/operations. Sustainable process synthesis–intensification, employed in this paper, is defined (Babi et al., 2014a) as the generation of alternative processing routes that show improvements related to economic factors, sustainability metrics and LCA factors.

Sustainable process synthesis-design can be achieved through the use of different methods (Halim et al., 2011; Smith et al., 2014; Tieri et al., 2014) that operate at the unit operations scale. However, three limitations exist. First, the use of hybrid/intensified unit operations is not considered. Second, the opportunity to innovate through the potential generation of novel unit operations is not provided because of the scale at which the methods operate. This opportunity is possible at the task scale (Siirola, 1996; Agreda et al., 1990) and phenomena scale (Lutze et al., 2013; Babi et al., 2014b, 2014c). Third, a comprehensive analysis, that is, an economic, sustainability and LCA analysis, are not used together for identifying design targets through the identification of process hot-spots. A process hot-spot are limitations/bottlenecks associated with tasks that may be targeted for overall process improvement. Therefore, by performing process synthesis–intensification, these three limitations can be overcome in a systematic manner.

In this paper a systematic, computer-aided, multi-stage, multi-scale framework for sustainable process synthesis–intensification that leads to the identification of more sustainable process design alternatives is presented. The framework is summarized in Fig. 1. In stage 1, that is, the synthesis stage, the problem is defined in terms of an objective function, subject to process constraints and performance criteria. A processing route is either found from a literature survey or generated from the application of the means-ends analysis (Siirola, 1996), thermodynamic insights (Jaksland et al., 1995) or superstructure network optimization (Zondervan et al., 2011; Grossmann, 2012). In stage 2, that is, the design stage, a base case design is first established and then analyzed in terms of economic factors, sustainability metrics and LCA factors for identification of process hot-spots. These process hot-spots are then translated into design targets that are to be satisfied if more sustainable alternatives are to be determined. In stage 3, that is, the innovation stage, desired tasks, phenomena, and the phenomena search space are identified (defined as design targets) and those desirable tasks and phenomena that may assist in overcoming the process hot-spots are identified. Process synthesis is applied using an integrated task-phenomena based approach in order to generate alternatives that achieve the design targets. Mutli-scale synthesis is possible because the base case design, in principle, can be decomposed from the unit operations scale to the task scale (Siirola, 1996) and phenomena scale (Lutze et al., 2013; Babi et al., 2014b). In the integrated task-phenomena based approach for process synthesis, phenomena are combined (rule-based) in such a manner that they perform a task or a set of tasks. These combinations of phenomena and/or tasks are then translated into unit operations using a knowledge-based, thereby leading more sustainable process designs or flowsheet alternatives. These designs are analyzed and compared to the base case design with respect to preselected performance criteria in order to determine the best, more sustainable process design.

Therefore multi-level synthesis is performed in the following manner. In stage 1, synthesis and design is performed in order to identify a feasible processing route that can be used as a base case in stages 2 and 3. In stage 2, task based synthesis is performed where, a task or set of tasks representing the function of a unit operation are identified and analyzed for generation of intensified flowsheet alternatives (task based). In stage 3, phenomena based synthesis is performed where, process phenomena are identified, analyzed and combined to generate flowsheet alternatives that are more sustainable and constitute of hybrid/intensified unit operations.

In this paper, the detailed architecture of the framework together with the main actions needed for successful application of each step of the work-flow is presented. An overview of the algorithms used in each step and the necessary methods and tools embedded within the framework are presented. The framework is applied to a case study of industrial importance, that is, the production of dimethyl-carbonate, where important features of the method of solution are highlighted.

2. Process synthesis–intensification: solution approach and definitions

The process synthesis–intensification problem is defined as follows (Babi et al., 2014b): For the production of a specified product, generate more sustainable process designs. These alternatives may include well-known, existing and novel hybrid/intensified unit operations that provide improvements in terms of efficient use of raw materials, sustainability metrics (impacts) as well as LCA factors compared to a reference (base case) design. The mathematical description is given in Section 2.1, the solution approach in Section 2.2, the concept of performing process intensification at different scales in Section 2.3 and the criteria for sustainability and LCA are explained in Section 2.4.

2.1. Mathematical formulation of the process synthesis–intensification problem

The problem definition for process synthesis–intensification is translated into a mathematical form:

$$\min/\max f_{obj}^{o} = f_{obj}^{o}(\underline{X}, \underline{Y}, \underline{d}, \underline{z}, \underline{\theta}) \tag{1}$$

subject to:

$$g(\underline{X}, \underline{z}, \underline{\theta}) \tag{2}$$

$$f(\underline{X}, \underline{Y}, \underline{d}, \underline{z}, \underline{\theta}) = 0 \tag{3}$$