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Publication date:
2019

Document Version
Publisher's PDF, also known as Version of record

A PHENOMENA-BASED SYNTHESIS METHOD FOR PROCESS INTENSIFICATION

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Abstract

Phenomena based synthesis is a process intensification (PI) method to generate innovative, more sustainable and non-trade off intensified and hybrid solutions. In the phenomena-based synthesis method, a target set of performance parameters is achieved using connectivity rules to combine phenomena at the lowest scale of aggregation directly affecting the driving force of a task or a set of tasks (Babi et al., 2015). Previously, this methodology was extended to include solid-liquid phenomena in order to widen the application range (Garg et al., 2018). In this research, the phenomena-based synthesis-intensification methodology is further developed and generalized to overcome the remaining application limitation and generate a wide range of solutions. New phenomena and their classes are introduced to expand the phenomena list. Furthermore, systematic algorithms based on thermodynamic insights are developed to identify desirable phenomena to combine in order to generate intensified/hybrid solutions. Thus, the presentation will showcase the generic phenomena based synthesis-intensification methodology, systematic steps and be illustrated with case-study examples.

Keywords

Process Intensification, Phenomena-based synthesis, Sustainable, Generic, Systematic

Introduction

In recent years, a major focus in process technology has been on hybrid/intensified and novel equipments that can dramatically improve the performance of chemical and biochemical processes. Therefore, tools, techniques and methodologies that potentially could transform basics of process synthesis and design; generating novel, innovative and sustainable solutions are highly desirable. The key attributes of such methods and tools should be that they are systematic, flexible in applicability and approach as well as covering a wide range of domains and scales from molecular to process or from phenomena to unit operation (unit-op) scale. There are numerous approaches developed in the past mainly categorized as knowledge-based methods (Siirola, 1996), methods based on mathematical optimization (Floudas, 1987) and hybrid methods (Babi et al., 2015) that combines different approaches into a single method. The objective of all these methods in one or other way is to generate better and more efficient solutions.

The phenomena-based synthesis method performs multi scale synthesis as it operates at unit-op, task and phenomena level. Thus, this approach is not limited to existing unit-ops and generates new and innovative solutions. In this short communication, an overview of the new phenomena-based synthesis intensification framework is presented along with the advances increasing the search space of unit-ops to generate innovative solutions.

Phenomena-based synthesis – general concepts

Most of the unit-ops constituting a chemical or a biochemical process can be represented in terms of mass, energy, momentum or transport phenomena. A list of such

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phenomena was developed by Lutze et al. (2012). These phenomena have been extended to incorporate a wider search space of unit-ops. An extended set of phenomena assists in generating new and innovative solutions which might be missing from the intensified solutions generated using the previous database. The new set of phenomena along with the possible classes is shown in Figure 1. Here, V represents vapor, L is liquid, S is solid, M is membrane while H, C and D within energy supply phenomena denotes heating, cooling and direct energy. Here direct energy supply ES(D) can represent any alternate energy source (e.g. microwave, ultrasound, centrifugal), other than cooling (C) or heating (H) that assists in enhancing a task or set of tasks within a given unit-op.

Phenomena Building Block	Class
Mixing (**M**)	V, L, S, VL, LS, VS
2 phase mixing (**2phM**)	LL, VL, LS, VS
Reaction (**R**)	V, L, S, VL, LS, VS
Energy supply (**ES**)	C, H, D
Phase contact (**PC**)	VL, LS, LL, VS
Phase transition (**PT**)	VL, LS, LL, VS, MVV, MLL, MVL
Phase Separation (**PS**)	VL, LS, VS, LL, VV, SS
Dividing (**D**)	-

Figure 1. Extended list of phenomena building blocks (PBB's) with different classes

The concept and examples of the extended phenomena list are shown in Figure 2, that otherwise could be a limitation. For example, if we consider the following phenomena, M(L)-mixing of liquid streams, R(L)-reaction in liquid phase and ES(D)-microwave energy source. The combination of these phenomena's generating a feasible simultaneous phenomena building block (SPB) performs a task that can be translated as a microwave reactor.

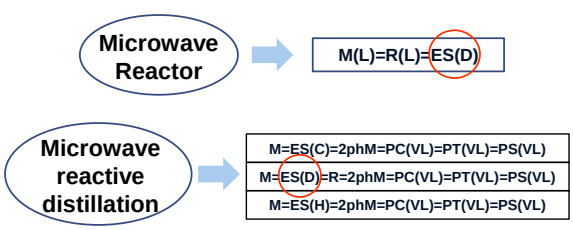

Figure 2. Unit-ops translating to phenomena

Likewise, the combination of two basic structures consisting of SPB's for a distillation and a microwave reactor forms a new basic structure that is translated to a microwave reactive distillation as shown in Figure 2.

An overview of phenomena-based synthesis framework

The generic framework to carry out phenomena-based synthesis-intensification consists of 3 steps including 10 sub steps. In step 1, the main objective is to identify the desirable tasks and phenomena that affect the driving force in the base case flowsheet and enables the methodology to have the potential of generating innovative and sustainable solutions. Here, an extensive database of unit-op and process hotspots translating to phenomena is used to carry out the respective sub steps.

In the second step, the feasible flowsheet alternatives are generated using developed algorithms, combination rules and feasibility rules. Here, a list of feasible simultaneous phenomena building blocks that performs a specific task are identified using thermodynamic based insights from Jaksland et al. (1995). Based on identified SPB's, the phenomena-based superstructure consists of feasible basic structures and is generated to identify flowsheet alternatives. The flowsheet options are reduced using logical and feasibility rules. Further, a detailed model based analysis and simulation is performed to identify the feasible flowsheet alternatives.

In the final step, feasible flowsheet alternatives are analyzed in terms of process economics, sustainability and life cycle indicators. The results for all the intensified alternatives are then compared with the base case through a set of pre-defined performance parameters.

For a flowsheet alternative to be non-trade-off and more sustainable, the selected performance parameters have to be either the same or better than the base case.

Conclusion

A new generic, systematic methodology has been developed to perform PI that operates at the lowest level of aggregation (phenomena) and generate a wide range of innovative and more sustainable solutions. The extended list of PBB's, databases and algorithms provides an increased search space to come up with an even wider range of solutions. Furthermore, incorporation of logical and feasibility rules makes the methodology more robust and quicker to generate feasible flowsheet alternatives.

In the presentation, the new step-by-step framework will be presented along with other advancements to carry out phenomena-based process synthesis intensification. The application of the framework will be demonstrated with different examples resulting in more economic and sustainable solutions.

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