Systematic Process Intensification

Salih Emre Demirel, Jianping Li, M. M. Faruque Hasan*

Artie McFerrin Department of Chemical Engineering, Texas A&M University

College Station, TX 77843-3122, USA.

Abstract

Process intensification often requires innovative equipment and flowsheets to achieve significant improvement compared to traditional unit operations. Systematic methods are needed for automatic generation, screening and discovery of promising intensification pathways at the conceptual design stage. In this contribution, we present a synopsis of the key elements of systematic process intensification (SPI), which include specification, representation, assessment, screening, and analysis. We conclude with a brief overview of future challenges and research opportunities in each of these areas.

1 Introduction

Increasing awareness for energy sustainability, environmental concerns, new and unconventional feedstocks, as well as recent advances in process optimization have sparked a renewed interest in process intensification (PI). PI combines reaction, separation, and other phenomena in multi-tasking units and reduces the cost, energy consumption, and footprint of chemical plants [1–9]. In the context of design, PI strives for innovative equipment and process configurations to overcome existing limitations through enhancing mass, heat and momentum transfer, decreasing equipment volumes and/or increasing efficiency while ensuring feasibility, operability, controllability and safety. Examples of PI technologies include reactive distillation, membrane reactor and task-integrated columns.

PI often requires innovation to generate "out-of-the-box" solutions to make drastic improvements - an area that is sometimes addressed through ad hoc considerations and heuristics. While optimization-based process synthesis methods can identify optimal configurations from a plethora

*Correspondence: Email: hasan@tamu.edu; Tel.: +1-979-862-1449

of alternatives, these alternatives need to be postulated and embedded *a priori* in a superstructure flowsheet. How to systematically generate and screen novel intensification opportunities remains an active area of PI research. In what follows, we summarize several key features of systematic process intensification, which encapsulates several recent developments in the field.

2 Elements of Systematic Process Intensification

Systematic process intensification (SPI) methods are equipped with computational tools and frameworks for generating and screening intensified process alternatives. Based on the methods that have been developed in the recent past, we can outline an SPI framework that typically consists of several steps. It often starts by defining the intensification problem at hand and gathering the necessary information as inputs (specification). One then provides a concise representation of all plausible intensification alternatives. In optimization-based approaches, this representation is typically obtained through a superstructure of process networks. Once we have a representation of equipment and process configurations, we employ one or several criteria for assessing the potential of different intensification pathways (assessment). Once an assessment criterion is fixed, we screen the set of alternative pathways to identify and rank the most promising ones (screening). Most promising alternatives are further analyzed in terms of their feasibility, operability, controllability and safety (analysis). While these steps are similar in nature to the ones considered in traditional conceptual design and process synthesis [11], SPI brings new methodological and computational challenges in these areas, some of which are elaborated further in the following sections.

2.1 Problem Specification

The scope of an intensification problem needs to be defined in terms of the products and raw materials specifications, available functional materials (e.g., solvents, separation agents, membranes, catalysts, etc.), design and operational constraints, physical and thermodynamic properties, parameter domains, and a list of possible reactions, phenomena and tasks that are associated with the problem. These specifications define the SPI search space. If the reactions are far from equilibrium or are accompanied by side reactions, one or multiple separation routes need to be considered to achieve the product specifications. We also need to provide a base case and a design configuration that can be used for benchmarking. Care needs to be taken for selecting the base case. If the base case represents a poor design, then even simple retrofits or integration may result in significant improvements, unnecessarily overemphasizing the success. Several methods

also rely on the base-case to analyze the process constituents to populate the pool of *building blocks* which are used in the subsequent stages of the design for process innovation and intensification [12–14]. Therefore, one needs to identify a base case that contains sufficient alternatives for task integration and phenomena intensification to achieve substantial improvement.

2.2 Representation

Representation methods are used to map various intensification alternatives so as to expedite the search for the best flowsheet candidates. A representation also determines the scope of the search space. Therefore, it is important to opt a representation that encapsulates as many potential intensification pathways (both intensified and classic) as possible. Several representations exist in the literature for process intensification, such as the generalized modular framework (GMF) representation [6,15], phenomena building block (PBB) representation [5,12,14], abstract building block representation [7,16], phenomena-based modular representation [17], and infinite dimensional state-space representation [18]. These representations encapsulate intensification alternatives at different levels, starting from representing fundamental driving forces to phenomena to tasks to unit operations to flowsheets. For instance, the generalized modular representation uses change in Gibbs free energy as fundamental driving force for transformation that occurs in reaction, separation and/or reactive separation modules. The phenomena-based approaches, on the other hand, consider both equilibrium-, transport- and kinetically-controlled phenomena that contribute to intensification. Lastly, traditional process synthesis representations, such as the unit operations-based [19], graph-theoretic [20] and task-based [4] representations, can be also used. However, generating new intensification alternatives are challenging using these representations, since they mostly focus on connecting unit operations at the flowsheet level.

In Figure 1, as an example, we illustrate the ABB representation. In a classic representation, an equipment hosts a single or multiple phenomena, such as reaction, phase contact, phase dividing, mixing, splitting, etc. A distillation column, for instance, can be viewed as a combination of several stages in each of which mixing, phase contact and transition between vapor and liquid phases takes place. Similarly, a membrane module can be viewed as combination of several stages of phase contact and transition phenomena that are governed by the diffusion through the barrier material that is placed between the retentate and permeate sides. A membrane reactor differs from a

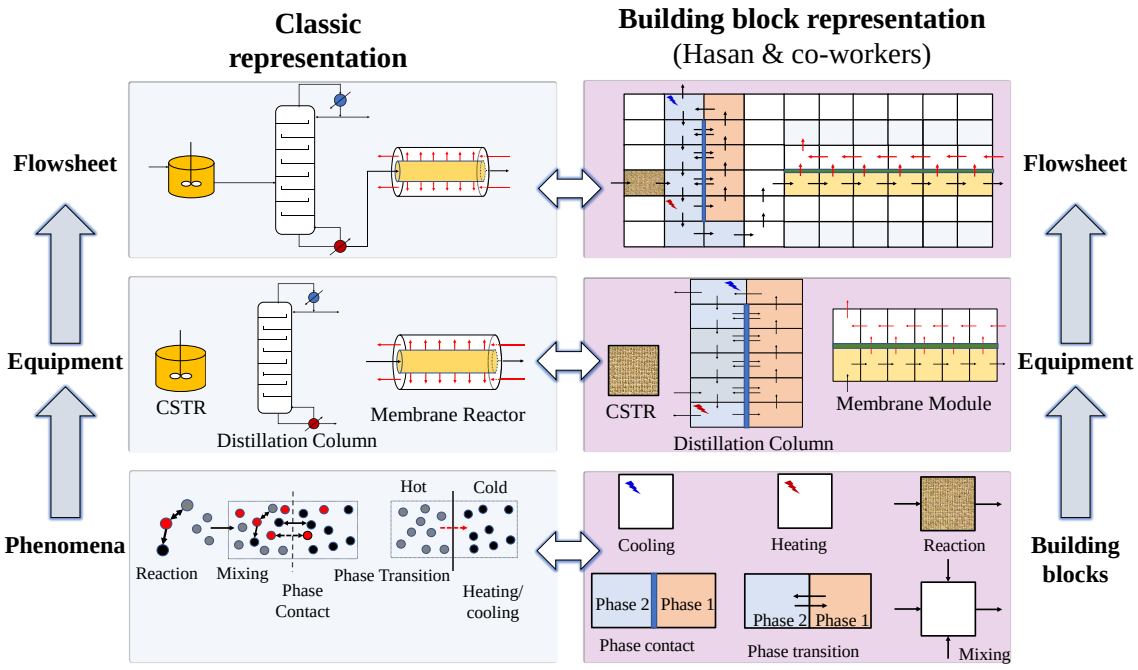

Figure 1. Classic and building block representations (Demirel et al., 2017) of chemical processes. The building block representation attempts to capture the phenomena descriptors even at the equipment and flowsheet levels. This allows a seamless transition from phenomena to task/equipment to flowsheets within a single framework, and makes it easy to incorporate various trade-offs and interactions among multiple competing phenomena at the conceptual design stage. Furthermore, the building blocks can be arranged in a two-dimensional "grid" superstructure to optimally assign the phenomena in single- and multi-functional units for systematic process intensification.

membrane module due to the presence of catalyst in one side. The building block representation in a two-dimensional grid, as proposed by Hasan and co-workers [7,15], departs from the classic approach and views a chemical process as a collection of abstract building blocks. As illustrated in Figure 1, each building block is an abstract module that can host different physicochemical phenomena. Each building block can be assigned a phase, temperature pressure and functionality (e.g., reaction). Furthermore, each of the four boundaries of a building block can have three possibilities. A boundary can be either unrestricted, semi-restricted, or completely restricted. An unrestricted boundary would allow unrestricted mass and energy exchange and represent complete mixing between two adjacent blocks. A completely restricted boundary would not allow any

exchange of mass and energy between neighboring blocks. A semi-restricted boundary, on the other hand, would allow selective passage, thereby enabling both equilibrium and kinetically-controlled mass and energy transfer.

Simple phenomena, such as heating, cooling, reaction, etc., can be represented using a single building block. Two neighboring blocks sharing a common semi-restricted boundary is used to represent others, e.g. phase contact, phase transition, a vapor-liquid equilibrium stage in a distillation column, a membrane compartment, a section of an absorption column, etc. In this case, the boundary assignment dictates the nature of the interaction between two blocks representing two phases. For instance, a semi-restricted boundary may represent an interfacial boundary between vapor-liquid phases (as in a distillation column tray or a rotating-packed bed), or it may stand for a physical barrier material (as in membrane separation). Combination of these fundamental building blocks paves the way for many different intensified/non-intensified equipment representations. A CSTR unit, for instance, can be represented by a single reaction block, a distillation column can be represented through combination of several vapor-liquid phase contact, transition and mixing blocks. Similarly, a membrane unit can be obtained through combination of a series of neighboring blocks separated by a common boundary which stands for the membrane material. If the blocks on the retentate side are assigned with reaction operation, a membrane reactor is obtained. When these building blocks are connected through inter-block streams, a complete flowsheet is obtained. This provides a systematic representation method for chemical processes.

Graphical representations are often used in the design of several chemical sub-systems, e.g. composition diagrams for non-ideal separator network synthesis [11], which are also extended to analysis of reactive distillation systems. Although useful in analyzing the feasibility under specific conditions, e.g., equilibrium limited reaction systems, these approaches alone also lack the innovative tools that SPI methods demand. Accordingly, more fundamental approaches have been proposed which rely on building blocks of the chemical processes, i.e. physicochemical phenomena [5,7,21,22] and processing tasks [4,23,24]. These methods are based on dissection of the available processing routes into smaller aggregations and investigate the possible design alternatives from the combination of these "*building blocks*" and/or enhancement of transport rates in these smaller processing route agglomerations.

2.3 Assessment

A promising intensified process should outperform the existing designs in at least one of the following aspects:

Equipment number and Size: Reduction in the number of equipment and size is a major end-results sought by systematic process intensification. Several works exist that addresses the reduction in number of equipment or their sizes [8,25,14, 26].

Energy consumption and Cost: Economics is often the main driver for widespread commercialization of new technologies. At the flowsheet level, intensification among various parts of a chemical process may require significant investment for mass and energy integration. At the equipment level, however, fixed capital investment may decrease with energy consumption and utility ratings. Therefore, minimization of energy consumption is often used as a means for generating intensified processes [7, 13] when the accurate cost functions cannot be specified beforehand. As a surrogate for the trade-offs between operating and capital costs, optimizing design variables (e.g., total reactive network reactive holdup and network capacity for reactive distillation systems [18]) are also considered as an objective in PI.

Environmental Footprint and Safety: Safety assessments are based on HAZOP (Hazard and Operability) and QRA (Quantitative Risk Analysis) methods which often require detailed design data. This poses challenges toward incorporating safety considerations at the early design stage. To this end, several safety metrics have been proposed [27]. Environmental footprint of process intensification can be measured through LCA (life cycle analysis) that quantifies impacts of the process and product throughout its lifetime [28].

Depending on the metric used, PI solutions differ. For instance, greater intensification of reaction and separation within a single compartment does not always correspond to safer and more efficient operation. To this end, a combination of intensification factors has been also proposed for screening and evaluating intensified alternatives [29].

2.4 Screening the Search Space

Systematic screening of feasible solutions is an integral part of obtaining intensified processes. There are several approaches for the synthesis of intensified processes: heuristic approaches [4,30], hybrid approaches [5, 31], and superstructure optimization-based approaches [7, 13]. Heuristic

methods rely on identification of hotspots and use of a set of guidelines to eliminate process bottlenecks. Hybrid methods use multi-step frameworks that combine heuristics and combination rules with optimization to sequentially reduce the search space for intensified alternatives. For instance, the phenomena-based methodology proposed by Gani and co-workers [5,12,21,32] performs both process synthesis and intensification in a hierarchical manner. The approach is able to identify the necessary and desirable phenomena and generate and screen various phenomena-based flowsheet options using a decomposition based solution strategy. The superstructure optimization-based approaches employ non-traditional representations which can be converted into mixed-integer nonlinear optimization (MINLP) formulations to identify optimal intensification routes and process flowsheets. GMF approach [6] seeks for promising intensified flowsheets through thermodynamically feasible mass/heat exchange modules. The building block superstructure [7] is constructed by positioning the building blocks in a two-dimensional grid. An assembly of blocks of the same type obtains a classical unit, while an assembly of blocks with different types results in an intensified unit. This allows to systematically identify and incorporate many intensification pathways in the building block superstructure. The overall problem is formulated using a single MINLP model that can be solved using commercial solvers.

2.5 Analysis

Process intensification often results in a loss of degrees of freedom [9]. Hence, the analyses of the implications of process intensification on process operability, controllability and safety are equally important. These analyses are generally performed after a pool of candidate intensified solutions is obtained and a dynamic model with appropriate fidelity is developed. Carrasco and Lima [33] proposed an optimization-based operability analysis for the intensification of modular process systems. Recently, Tian et al. [34] proposed an integrated framework for the synthesis of operable intensified systems based on generating candidate flowsheets using the GMF representation and further analyzed the resultant designs for operability and safety.

3 Challenges and Future Opportunities

Although significant work has been done in recent years in the area of systematic process intensification, there remains several challenges and research opportunities. Some of these are discussed as follows.

At the molecular level, systematic methods are required to elucidate the various trade-offs and interactions between multiple competing phenomena involved in intensification. The equilibrium, transport and kinetic properties of functional materials (e.g., solvents, catalysts, adsorbents) influence intensification. Furthermore, a process can be intensified using a single material with multiple functionalities, or using multiple materials with single functionality [35]. Often it is not clear how a combination of materials could intensify the process-level performance. Fundamental understanding of these knowledge-gaps will facilitate the design and control of intensified processes. Opportunities exist in developing multiscale systems engineering methods and tools to elucidate the influence of material properties on process intensification, and develop fundamental modeling and design rules and recipes.

At the equipment level, it remains a challenge to obtain reliable cost parameters and formalize appropriate cost functions for novel and intensified designs. While phenomena-based approaches are able to create new (and often exotic) unit operations, it is difficult to systematically decide on the boundaries of new intensified equipment.

At the process level, the currently available flowsheet simulators are based on modular design concepts which limit their applicability for novel equipment configuration and process intensification. Computer-aided tools are needed for integrating the recent advances in process synthesis with innovative design capabilities to automatically generate intensified process flowsheets. Existing sequential solution strategies often limit the search space for novel intensification pathways. Superstructure-based simultaneous approaches, on the other hand, are limited by the rigor, accuracy and complexity of the underlying models used for optimization. Furthermore, safety and economic objectives are often in conflict with each other and are challenging to address in a single optimization framework. To this end, multi-objective optimization can generate a pool of decisions while appropriately considering the trade-offs between the conflicting objectives [36].

In many cases, intensification can be also achieved through exploiting process dynamics and periodicity (e.g., sorption-enhanced reaction process, simulated moving bed, cyclic distillation, etc.) [37]. Optimization of cyclic processes requires solving dynamic, complex and high-fidelity models [38–41]. Although attempts have been made for consideration of batch and continuous operation in reactor networks [42], there is still a significant disconnect between the steady-state

and the dynamic approaches. Furthermore, intensification may induce new challenges in process dynamics and control [43]. Lastly, opportunities exist for systematic process intensification methods to discover innovative processes for application areas beyond the traditional chemical sector, such as integrated biorefinery, pharmaceuticals and semiconductor industry.

4 Concluding Remarks

Systematic process intensification (SPI) methods play important roles in generating energy-efficient, cost-effective and sustainable designs for the chemical industry. The recent developments in SPI methodologies have been catalyzed by increased competitions in the global market and societal awareness toward more sustainable production routes. The key steps in SPI include problem specification, representation, screening the search space and analysis of solutions. Outstanding challenges in SPI include incorporation of (i) property prediction and material selection in a multi-scale optimization framework, (ii) accurate cost functions for novel technologies, (iii) safety, controllability and operability features, (iv) dynamic/cyclic operation synthesis, (v) effective simultaneous solution strategies for identification of the intensified equipment and flowsheet synthesis, and (vi) software platforms where intensified systems can be generated and validated through detailed models. Addressing these problems will ignite a new era for chemical industry marked with widespread realization of more efficient, sustainable and safer production concepts through process intensification principles.

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Conflict of Interest

The authors declare no conflict of interest.

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