Computers and Chemical Engineering 81 (2015) 130–137

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

A perspective on process synthesis: Challenges and prospects

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ARTICLE INFO

Article history:
Received 29 November 2014
Received in revised form 28 April 2015
Accepted 7 May 2015
Available online 15 May 2015

Keywords:
Process synthesis
Distillation sequences
Separation systems
Surrogate models

ABSTRACT

This paper gives the author's perspective on some of the open questions and opportunities in process synthesis focusing on separation systems as the application. Driven by energy and environmental concerns and challenged by introduction of new raw materials, this author anticipates significant advances in: (1) novel approaches that integrate experimental studies and process synthesis activities, and multi-scale and surrogate models for accurately capturing the behavior of these unconventional mixtures, (2) systematic generation of alternatives for processing these mixtures, and (3) global, robust, and stochastic optimization for identifying the optimum alternative. This paper is an extended version of a conference paper (Cremaschi, 2014) presented at the 8th International Conference on Foundations of Computer-Aided Process Design.

1. Introduction

Since the introduction of the term "process synthesis" in the late 1960s, the process systems engineering (PSE) community made significant progress in the area. As depicted in Fig. 1, for given desired products and available raw materials, the process synthesis methods try to determine the combination of processes to obtain the products starting from the raw materials while satisfying a predetermined objective, which is in most cases minimum cost, but may also be minimum energy consumption or maximum yield among others. One of the author's favorite quotes by Westerberg (2004) about process synthesis reads as follows: "Process synthesis is very much the fun part of engineering. It is where one invents the structure and operating levels for a new chemical manufacturing process."

The first review in process synthesis by Hendry et al. (1973) had over 60 articles. The 12th Annual Symposium on Computer Applications in Chemical Engineering had 10 contributed papers in process synthesis area – three dealing with heat exchanger networks, two in synthesis of separator networks, four in overall flowsheet synthesis, and one industrial experience paper that discussed the application of the existing synthesis approaches to heat exchanger, separator, and reactor networks – out of 115 overall contributions (Motard, 1979). A recent search in the abstract and citation database Scopus yielded well over 2000 publications from 1972 to 2013. Fig. 2 shows the annual number of publications in the four main areas that our community focused on over the last four decades: reactor network, distillation train, heat-exchanger network, and overall flowsheet synthesis. Fig. 2 suggests at least a linear increase in the total number of publications in the process synthesis area over the last two decades, a little over half of the contributions in heat-exchanger network synthesis, followed by contributions in separator sequence and overall flowsheet synthesis.

Clearly, a review of the existing literature in this paper is neither feasible nor the intent. However, the author refers the interested reader to a selected subset of excellent reviews and perspective papers on: reactor and reactor-separator network synthesis focusing on attainable region construction (Feinberg, 2002), synthesis of heat integration networks (Furman and Sahinidis, 2004; Morar and Agachi, 2010), water network synthesis (Jeżowski, 2010), distillation-based separation sequence synthesis (Skiborowski et al., 2013), and general process synthesis approaches focusing on their substantial potential for synthesis of sustainable and environmentally-friendly processes for energy and chemicals production (Grossmann and Guillén-Gosálbez, 2010; Yuan and Chen, 2012; Yuan et al., 2013).

The goal of this paper is to provide the author's perspective on some of the open issues as they relate to process synthesis using separation-system synthesis as an example domain. It is this author's opinion that process synthesis holds unique potential to contribute to the solution of some of the "Grand Challenges for Engineers" identified by National Academy of Engineering, and separation systems will play a vital role for addressing energy, water, and pharmaceutical needs, and carbon capture problems. A brief overview of process synthesis approaches is given in next section.

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http://dx.doi.org/10.1016/j.compchemeng.2015.05.007
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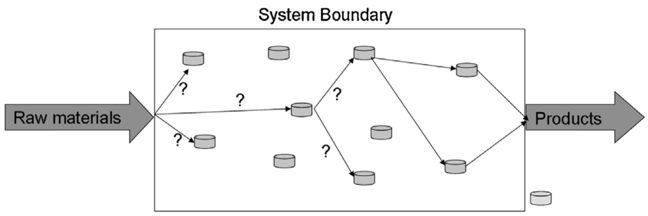

Fig. 1. A graphical representation of process synthesis.

Section 3 discusses open issues and opportunities in separation-systems synthesis. The last section offers concluding remarks.

2. Process synthesis approaches

The approaches used to address process synthesis problems can be categorized into one of the two broad groups: (1) hierarchical decomposition based heuristic approaches, and (2) mathematical programming based approaches. The early contributions to the process synthesis area were mostly development and implementation of systematic hierarchical decomposition approaches to remove the chemical and physical differences between the raw materials and the products, e.g., means-ends analysis (Siirola and Rudd, 1971), and the 5-level decision hierarchy to conceptual design (Douglas, 1988). The economic short-cut evaluations of the alternatives were carried out at each decision level to reduce the number of alternative flowsheets. Although powerful and generally yielding near-optimal processes, the heuristic based decomposition approaches do not consider the interactions between different levels, and cannot guarantee that the end design is the best possible for the selected performance metric, mostly an economical one.

Tied mostly to increasing computing power and advances in formal optimization techniques, mathematical programming approaches, i.e., superstructure optimization, were developed to incorporate the interactions between different design levels and their overall effect on the selected performance metric. In superstructure optimization, the overall process network is determined in one simultaneous mathematical programming problem by optimizing a desired performance metric given the initial superstructure of the system, the material flow through each interconnection, operating conditions, and other design parameters for each equipment (Barnicki and Siirola, 2004).

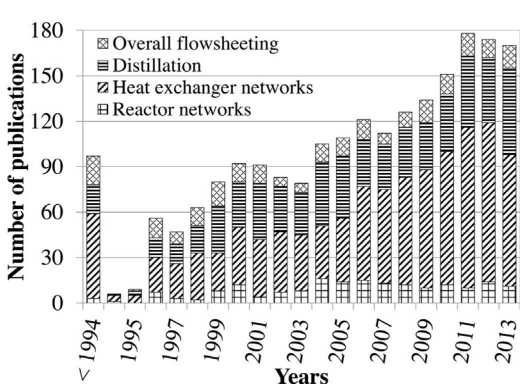

Fig. 2. Number of process synthesis publications (1972–2013) – reactor networks: search in All Fields for the exact phrase "reactor network synthesis", distillation: search in All Fields for either of the following exact phrases "distillation column synthesis", "separation network synthesis", "distillation sequence synthesis", "distillation synthesis", "separation train synthesis", heat-exchanger networks: search in All Fields for the exact phrase "heat exchanger network synthesis", and overall flowsheeting: search in All Fields for either of the following exact phrases "flowsheet synthesis", "complete flowsheet synthesis", "general flowsheet synthesis".

The first step in superstructure optimization is to construct a map of all the design alternatives using an appropriate representation. The commonly used representations for process synthesis problems are State-Task, State-Equipment, and Resource-Task Networks, and Generalized Modular Framework. More recently, Unit-Operation-Port-Stock Superstructure and group-contribution based representations are proposed. A brief review of these representations can be found in Fahmi et al. (2014). Once the alternatives are mapped, the next step is to translate this representation to a mathematical programming formulation, mostly resulting in a large-scale nonconvex mixed integer (non)linear programming (MINLP) problem, whose objective is generally an economic one.

The resulting optimization formulation, in most cases very difficult to solve, fostered the development of a myriad of tailored and general optimization algorithms, e.g., the outer-approximation approach for obtaining local solutions (Viswanathan and Grossmann, 1990), and BARON – Branch-And-Reduce Optimization Navigator – (Tawarmalani and Sahinidis, 2005), or ANTIGONE – Algorithms for coNTinuous/Integer Global Optimization of Nonlinear Equations – (Misener and Floudas, 2014) for obtaining global solutions. Although superstructure optimization is theoretically a very powerful approach, its penetration to the industrial applications has been limited due to two major drawbacks: (1) the optimum can only be obtained if the superstructure contains the optimum when constructed (Barnicki and Siirola, 2004), (2) the difficulty of solving the resulting MINLPs (Henao and Maravelias, 2010). Both decomposition-based and mathematical programming approaches have their own limitations, and their strengths may be complementary. Some of the recent contributions focus on combining these approaches for synergistic effects (Yuan et al., 2013).

3. Challenges and opportunities – separation-system synthesis

Top chemical companies are shifting their focus from bulk chemicals to specialty products. For example, BASF expects to increase the share of "customized products, and functionalized materials and solutions" sales to 70% of its total by year 2020. They continue to acquire specialized "close-to-end-user" businesses as they exit from some of the commodity markets (e.g., fertilizers) (BASF, 2014). In a similar trend, the Dow Chemical Company is "carving-out" its chlorine and epoxy assets reducing its commodity chemicals foot-print while it continues to grow in downstream specialty products in integrated plastics, electronics, and agriculture (Dow Chemical Company, 2014). Bayer recently announced that they will become a "pure Life Science company", focusing their business entirely on products that enhance human health and nutrition (Bayer, 2014). Dupont continues to focus its product offerings on agriculture and nutrition developed using the latest advancements in biotechnology (DuPont, 2013). These trends suggest that the raw material and product portfolios of chemical process industry may grow and be quite different compared to today's in the near future.

The world population is expected to grow to 9 million by 2050 causing considerable increases in energy and natural resource demands. Based on the report titled Environmental Outlook to 2050 by The Organization for Economic Co-operation and Development (OECD), the world's economy is expected to grow four times its current size using 80% more energy by 2050. The climate change due to increased greenhouse gas emissions from economic growth, loss of biodiversity, water scarcity, and substantial increases in SO_x and NO_x emissions in developing economies are identified as