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A review on superstructure optimization approaches in process system engineering

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ABSTRACT

In this paper, we survey the main superstructure-based approaches in process system engineering, with a particular emphasis on the existing literature for automated superstructure generation. We examine both classical and more recent representations in terms of generality, ease of use, and tractability. We also discuss the implications that different representations may have on strategies for algebraic modeling and optimization. We then review the state-of-the-art in software implementations to support synthesis. Finally, we examine the use of evolutionary—recently referred to as superstructure-free—approaches, in which algorithmic procedures dynamically generate and evaluate candidate process structures.

1. Introduction

Conceptual process design is a central pillar of chemical engineering, concerning the definition, simulation, optimization, and control of chemical processes. This design task involves the synthesis of complex chemical processes through the integration of simpler unit blocks characterized by physical and chemical properties. Methodological developments in process synthesis have been addressed by the Process Systems Engineering (PSE) community (Klatt and Marquardt, 2009; Cremaschi, 2015; Grossmann and Harjunkoski, 2019), which has developed powerful mathematical optimization and simulation tools to address chemical process design and control problems. In particular, Mixed-Integer Nonlinear Programming (MINLP) and Generalized Disjunctive Programming (GDP) techniques are well-suited to problems involving selection among discrete process alternatives with nonlinear process phenomena (Grossmann, 1989; Grossmann et al., 2000; Grossmann, 2002; Trespalacios and Grossmann, 2014; Chen and Grossmann, 2019).

Two main approaches exist for conceptual process design: hierarchical decomposition (Douglas, 1985; Siirola and Rudd, 1971) and superstructure synthesis (Umeda et al., 1972; Chen and Grossmann, 2017), with superstructure synthesis preferred for its systematic evaluation of a large space of structural alternatives (Saif et al., 2009; Barnicki and Siirola, 2004; Westerberg, 2004). Hierarchical decomposition involves a sequential procedure in which the process design is progressively defined in stages (or levels). At each level, specific decisions are made based on engineering judgement and rules-of-thumb, starting with broader decisions of the greatest consequence. For detailed reviews on hierarchical decomposition approaches see the works of Dimian (2003) and Goh and Ng (2015). However, interactions between decisions at different detail levels (e.g. separation design and heat integration) are difficult to capture with hierarchical decomposition (Duran and Grossmann, 1986b; Lang et al., 1988). In contrast, superstructure synthesis attempts to solve the simultaneous design problem as a mathematical programming problem. Hybrid approaches combining ideas from both hierarchical decomposition and mathematical programming have also been studied by Daichendt and Grossmann (1997) and more recently by Zhang et al. (2016). Targeting techniques are also available, which identify *a priori* characteristics of advantageous structures by analyzing physical properties of the chemical system; these have been applied to great effect in heat exchanger networks (Linnhoff and Hindmarsh, 1983; Hohman, 1971), and in heat and water integration (Klemeš and Kravanja, 2013). The composite curves diagram in pinch analysis (Linnhoff and Hindmarsh, 1983) and the attainable region-based methods, introduced by Horn (1964) and popularized by Glasser et al. (1987), are among the most notable targeting techniques, used in the design of heat exchanger networks and reaction-separation systems. More recent contributions by Feinberg and Ellison (2001) and Frumkin and Doherty (2018) extend ideas of the latter beyond their geometric origins.

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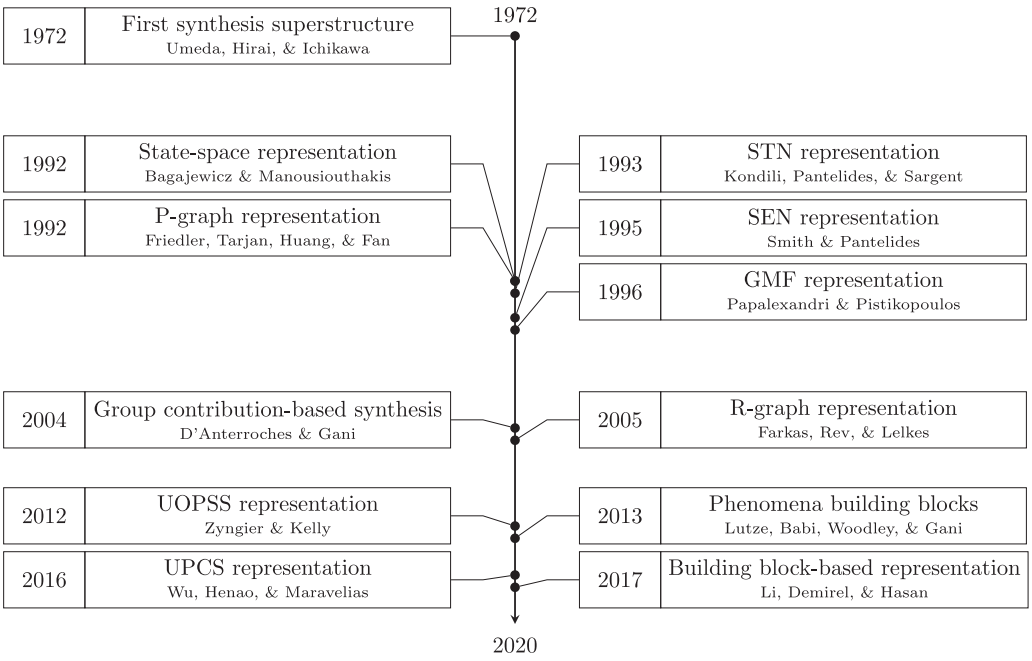

Fig. 1. Abbreviated timeline of superstructure synthesis representations.

Superstructure-based process synthesis, introduced in Umeda et al. (1972), involves three main sequential steps: (i) the postulation of a superstructure, which encapsulates the set of all feasible alternative process structures; (ii) the translation of the superstructure into a mathematical programming model; and (iii) the computation of an optimal structure by solving the mathematical optimization model. The approach gained traction first in subsystems (Sargent and Gaminibandara, 1976; Grossmann and Sargent, 1976), then in general flowsheet design (Kocis and Grossmann, 1989). Early reviews in the area can be found by Nishida et al. (1981), Westerberg (1991), and Bagajewicz and Manousiouthakis (1992).

An inherent limitation of superstructure-based approaches is the need to define an initial superstructure to capture all the desired alternatives. A poorly-constructed superstructure may omit several feasible or optimal process flowsheets. Moreover, the choice of representation may impact tractability of the resulting optimization formulation (Yeomans and Grossmann, 1999). In response, the community has developed two main approaches: (a) automated superstructure generation methods, and (b) evolutionary "superstructure-free" approaches. In automated superstructure generation, the superstructure is constructed from a set of alternatives via deterministic algorithmic procedures; on the contrary, in the superstructure-free approach, candidate structures are dynamically generated during the search process.

In this paper, we provide a critical review of the state-of-the-art in superstructure based synthesis, with a focus on the methods and tools available to generate appropriate superstructure representations. We then compare these approaches to superstructure-free design strategies. The rest of the paper is organized as follows. In Section 2, we survey the representations and algorithmic procedures proposed in the literature to automate the generation of the superstructure of a given process. We also describe algorithmic post-processing procedures proposed to reduce the complexity or the redundancy of superstructure representations, and to translate the superstructure into a mathematical programming formulation. In Section 3, we discuss implications of the superstructure representation on modeling and solution strategies. In Section 4, we review current software implementations for process synthesis. Then, in Section 5, we briefly summarize superstructure-free approaches. Methodological conclusions and final remarks follow in Section 6.

2. Superstructure representations

In this section we present the different techniques proposed in the literature to generate and optimize the superstructure of a given chemical process. Selection of the appropriate superstructure representation is a necessary prerequisite in automated superstructure generation. Over the years, several representations and generation approaches have been proposed in literature (see Fig. 1); these can be divided into two classes: the traditional approaches proposed in the 1990s, and newer representations developed after the turn of the millennium. The traditional approaches involve network or graph representations in which the chemical process is divided into stages (or states) and tasks. These interlinked states and tasks describe the progressive transformation of the inputs (or raw materials) into the desired outputs (or final products) by means of sequential operations (or functions). Computer-aided generation of alternatives in these approaches can be done with means-ends analysis (Siirola et al., 1971).

In recent years, new challenges and opportunities—detailed in the following review papers—have spurred renewed interest in process design, leading to the development of several new superstructure representations. There have been efforts to design more sustainable processes (Martín and Adams II, 2019) for the circular economy (Avraamidou et al., 2020). Interest in process intensification renewed interest in representations able to capture selection and integration of physical and chemical phenomena, in contrast to traditional equipment-oriented superstructures (Sitter et al., 2019; Tula et al., 2019a; Tian et al., 2018a). At the same time, equipment size reductions from process intensification have led to interest in modular process units (Baldea et al., 2017), with applications in the oil and gas industry (Tsay et al., 2018). New superstructures that aim to simplify solution strategies and software platforms to support the use of these new representations have also arisen (Mitsos et al., 2018; Tula et al., 2019b). Finally, Ryu et al. (2020) explicitly examines the interactions needed to synthesize a process em-

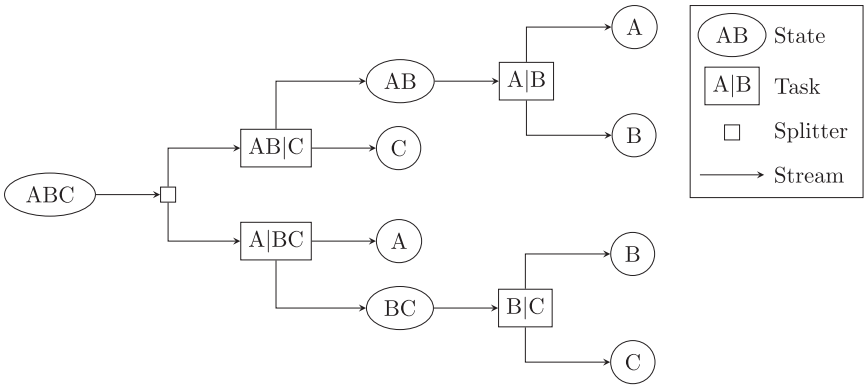

Fig. 2. State-Task Network (STN) superstructure for a 3 component sharp split distillation sequence.

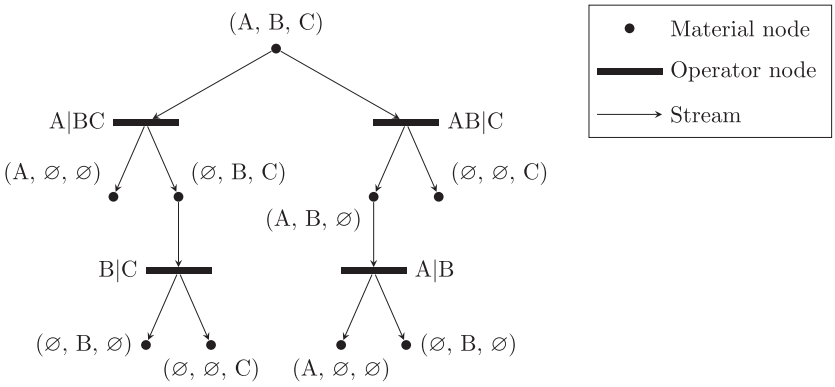

Fig. 3. P-graph network superstructure (PNS) for a 3 component sharp split distillation sequence.

bedding multiple different representations. In the following subsections, we elaborate on both traditional and new representations and the tools available for their automatic generation. A summary of case studies investigated using these representations can be found in Appendix A, Table A.2.

2.1. State-task network representation

The state-task network (STN) representation (see Fig. 2) was first introduced in Kondili et al. (1993) for multi-product/multi-purpose scheduling problems, and extended to process flowsheet design by Yeomans and Grossmann (1999), in which the representation is applied to the synthesis of distillation sequences with and without heat integration. The STN representation consists of a directed graph with two main classes of nodes: states and tasks. States, as their name implies, represent a physical or compositional state of the feeds, intermediates, or products. The transition between these states is accomplished through processing tasks. A superstructure task can be conditional or common to all the alternative structures; this distinction is only made when the superstructure is translated into a mathematical programming formulation.

For conceptual design, the processing tasks also need to be associated with equipment selection. Due to its origins as a multi-product scheduling representation, the STN supports variable task-equipment (VTE) assignment, in addition to the more traditional one task-one equipment (OTOE) assignment. In VTE, a single piece of equipment may perform multiple different processing tasks (e.g. batch reactors that perform both reaction and mixing tasks), and the final equipment-task assignment is given by the optimization result. However, OTOE is far more common in overall flowsheet design, with each task associated *a priori* to a piece of equipment. In that way, the superstructure more closely resembles a process flow diagram with conditional flow paths. The STN-OTOE representation is still commonly used today, and has inspired new representations that build on its ideas. As previously introduced, the STN can be constructed by taking into account all of the tasks needed to convert a process through means-ends analysis (Siirola et al., 1971), and connecting them via associated intermediate states.

2.2. P-Graph representation

The process graph (P-graph) concept first appeared in Friedler et al. (1992a). As such, it is a contemporary to the STN, with many similarities between the two representations. The P-graph is a bipartite graph (see Fig. 3), whose vertices consist of material (M-type) and operating unit (O-type) nodes. An operating unit accepts one or multiple input materials, and produces one or more outputs. P-graph material nodes correspond to STN state nodes; P-graph operating units, to STN tasks.

Drawing upon ideas from graph theory, Friedler et al. (1992b) show that combinatorially feasible process structures are subgraphs of the P-graph that satisfy the following system of axioms.

Axiom S1. Every final product of the process is represented by a M-type vertex in the graph.

Axiom S2. A M-type vertex represents a raw material, if and only if it has no incoming incident arcs.

Axiom S3. Every operating unit defined in the synthesis problem corresponds to an O-type vertex in the graph.

Axiom S4. There exists at least one path from each operation unit node to a node representing a final product.

Axiom S5. Every material node should represent an input or an output to/from at least one operating unit node.

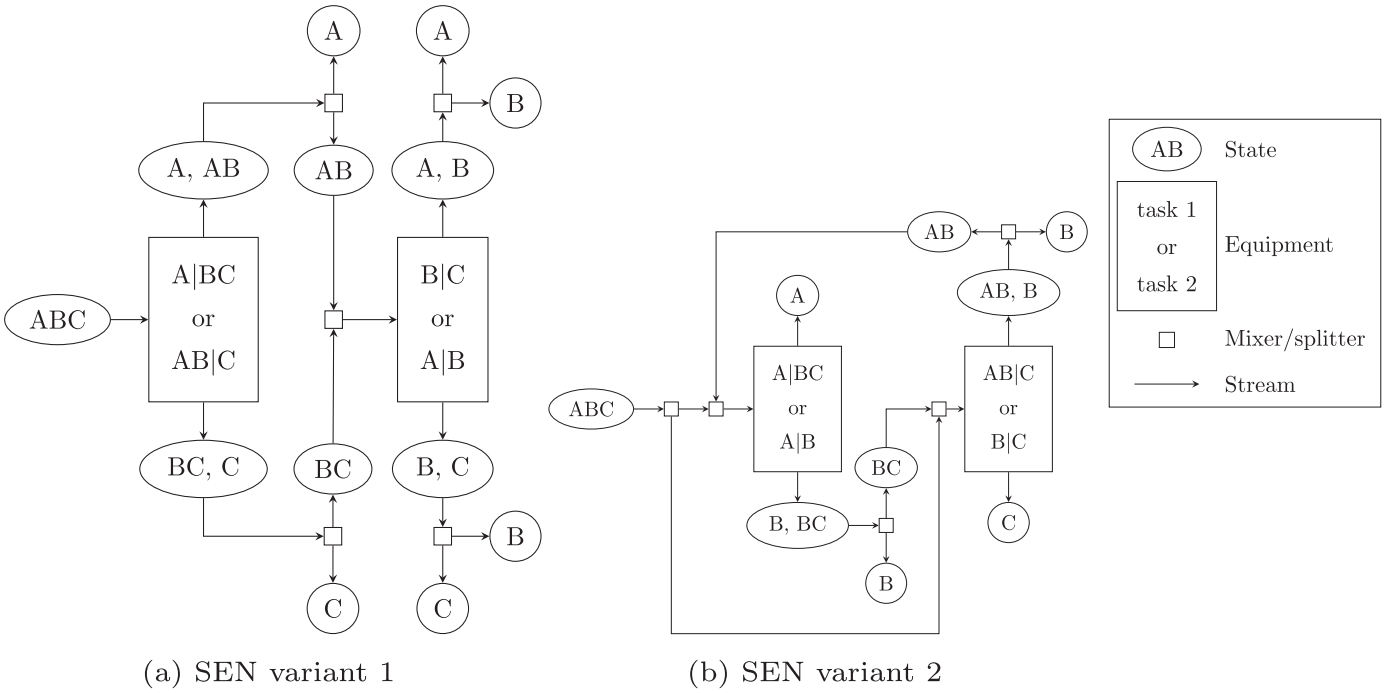

Fig. 4. State-Equipment Network (SEN) superstructure for a 3 component sharp split distillation sequence.

Axiom S1 ensures that all desired products appear in the superstructure, while Axiom S2 defines which nodes are the raw material input nodes. Axiom S3 ensures that all considered operating units appear in the graph. Axiom S4 requires that each operating unit be connected to at least one final product, i.e. there are no irrelevant operations. Finally, Axiom S5 enforces that every material node is connected to at least one operating unit node, i.e. there are no irrelevant materials. The set of structures described by these axioms is closed under union, and the superstructure corresponds to the union of all the structures.

The P-graph methodology distinguishes itself among early superstructure representations by providing a systematic algorithm for generating the P-graph (Friedler et al., 1993). The computational complexity of this algorithm is polynomial in the number of the materials and in the maximal degree of its vertices (Friedler et al., 1993). An accelerated branch-and-bound (ABB) strategy was also developed to exploit the P-graph representation by restricting the search to combinatorially feasible structures and solving the relaxations at branched nodes in reduced space (Friedler et al., 1996). It is noteworthy that contemporary to this, the same motivations guided development of the logic-based outer approximation algorithm for Generalized Disjunctive Programming (Türkay and Grossmann, 1996) (see also Section 3.3). Connections between the P-graph representation and GDP formulations were subsequently explored in Brendel et al. (2000).

The mathematical rigor unpinning the P-graph methodology is a key advantage of the approach; however, its closed implementation and complex notation limit its accessibility to a chemical engineering audience. For more detail, recent reviews on the P-graph approach may be found by Lam (2013) and Friedler et al. (2019).

2.3. State-equipment network representation

In the state-equipment network (SEN) representation (see Fig. 4), introduced by Smith and Pantelides (1995), the superstructure nodes are states and equipment, with task assignment to the equipment determined as an optimization result. For some problem classes, e.g. distillation sequence design, SEN requires fewer operator (equipment/task) nodes than the equivalent STN representation. For a three-component system with sharp separations, the SEN requires two equipment nodes versus four task nodes for the STN; for a four-component system, the ratio is four to 10 for the SEN and STN, respectively. However, with the SEN, the combinatorial complexity is found in the equipment interconnections, so it is more effective when the equipment selection is known *a priori* (Yeomans and Grossmann, 1999), as in distillation sequences and reactor selection (Ramapriya et al., 2018).

Note that multiple logically-equivalent SEN variants may be possible with differing assignment of potential tasks to the equipment, as seen in Section 2.3 for a distillation sequence superstructure. Variant 1 (Fig. 4a) has a more intuitive flow pattern, with the first separation taking place in the first column, and the second separation taking place in the second column. Variant 2 (Fig. 4b) groups the tasks by the split taking place, with the A|B separation in the first column, and the B|C separation in the second column. As a result, variant 2 potentially has less physical property variation between discrete task selections at either the condenser or reboiler end of the column, with a high concentration of the same pure component. This could improve computational performance in optimization algorithms. The relative merits of these two variants remains an open question.

Related to both the STN and SEN is the Resource-Task Network (RTN) representation, introduced by Pantelides (1994), in which the resource nodes can refer to material states (as in the STN) and/or equipment (as in the SEN). The RTN is more common in process scheduling applications, but can be useful in simultaneous scheduling and design problems. We omit a detailed discussion here and refer the interested reader to recent reviews on scheduling formulations (Harjunkoski et al., 2014; Brunaud et al., 2020).

The recent Processing Step-Interval Network, proposed by Bertran et al. (2016), can also be seen as an extension of the STN/SEN, with influence from early heat exchanger network models (Yee and Grossmann, 1990). The representation adds structure and nuance to the states through the use of processing intervals. An example of its use can be found in Garg et al. (2019) for the production bio-succinic acid.

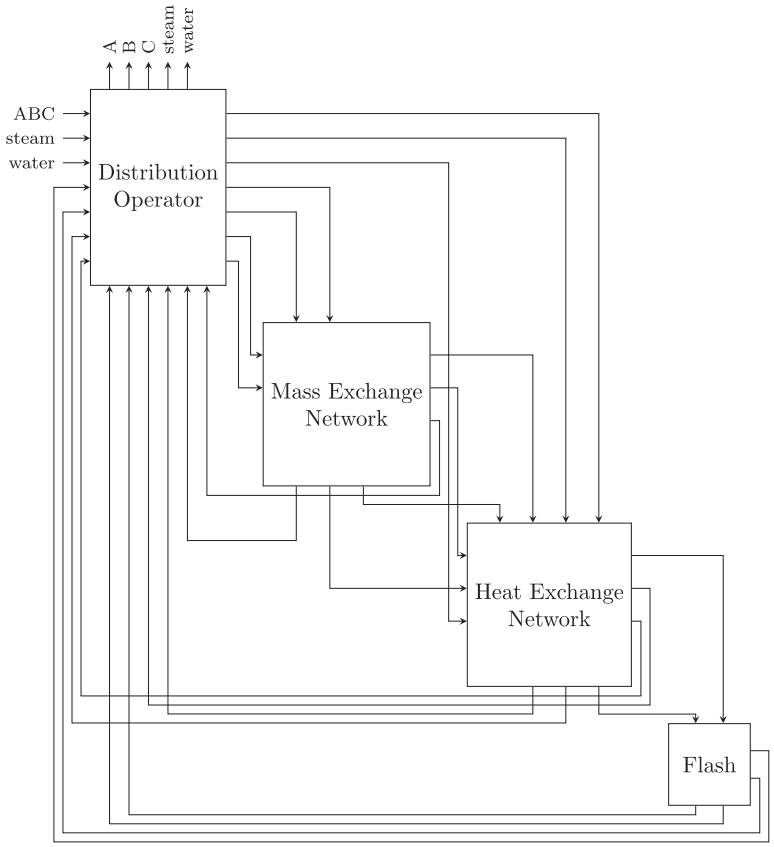

Fig. 5. State-Space Representation (SSR) superstructure for a 3 component sharp split distillation sequence. Boxes represent state-space operators. Arrows represent state variables that are inputs to or outputs from their respective operators.

2.4. State-space representation

The state-space representation (SSR) was adapted from the concept of "state space" in system theory (Zadeh and Desoer, 1979). In the state-space approach, the design problem is posed as identification of the properties of the input-state-output relations between input and output variables (Bagajewicz and Manousiouthakis, 1992). The input/output variables are defined by the process engineer, while the input-state-output relations between variables yield a given structure. For process synthesis, the structure involves sequential applications of two classes of functions, namely (a) mixing and splitting of streams in the distribution network, and (b) unit operations which determine the process operator.

The SSR was motivated by the ability to easily generate complex distillation configurations such as Petlyuk columns. In Bagajewicz and Manousiouthakis (1992), the SSR for a distillation network is introduced as the integration of heat- and mass-exchanger operations. The state space approach was further extended by Wilson and Manousiouthakis (2000), which explores the limits of discretization of the design space. Another similarly-motivated extension was recently developed by Liesche et al. (2019).

The SSR is characterized by matrix operations involving the state variables. The numerical structure of these matrix operators ultimately translates to a physical process structure. Visualization of the SSR (see Fig. 5) involves abstract boxes representing the operators, interconnected by the state variables serving as inputs to or outputs from these operators. The mathematical convenience of the matrix-operator interpretation has gained the SSR significant popularity in process integration (mass/heat/work exchange) applications (see Table A.2). In Saif et al. (2009), a comprehensive survey on the applications of the SSR methodology to optimization of membrane and hybrid membrane process systems for wastewater treatment is presented.

The SSR is a very general representation, but given its abstractness and lack of supporting software tools, it has seen limited uptake outside of its proven area of process integration.

2.5. R-graph representation

Farkas et al. (2005b,c) adapt the SEN-OTOE to create the R-graph representation (see Fig. 6), in which nodes correspond to the inlet and outlet ports of each candidate process unit. The inlet ports function as multi-stream mixers, while the outlet ports correspond to splitters. Directed edges between the ports represent process streams, which always originate from an outlet port and end at an inlet port. The R-graph representation also features source and sink units, corresponding to raw materials and products, respectively. The source unit only has an outlet port, while the sink unit only has an inlet port. By definition, all R-graph nodes must be connected to another node in the graph.

The R-graph is motivated by modeling concerns that may arise in the traditional STN or SEN approach. First is the problem of multiplicity and redundancy, whereby a superstructure encodes multiple equivalent solutions, needlessly increasing the computational cost of the search algorithm. These redundant structures are easily created when unit bypasses are possible. In addition, no unique algebraic description is generally available for a given superstructure. Simple algebraic transformations can give rise to an infinite number of mathematical programming formulations that all yield the same engineering solution.

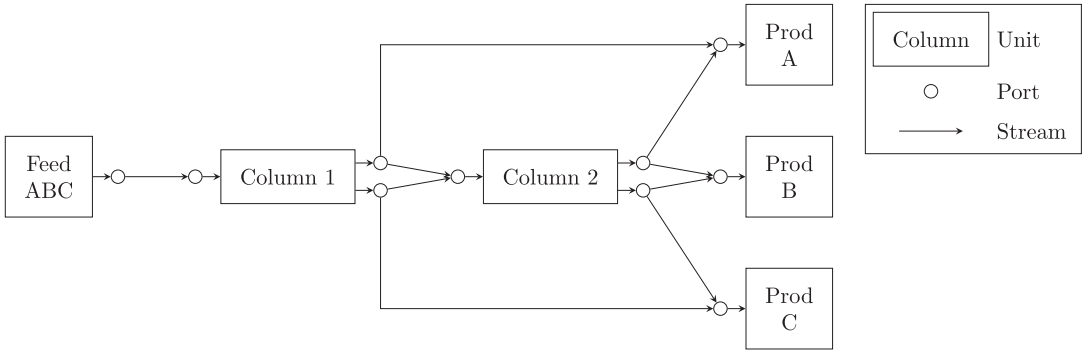

Fig. 6. R-graph superstructure for a 3 component sharp split distillation sequence.

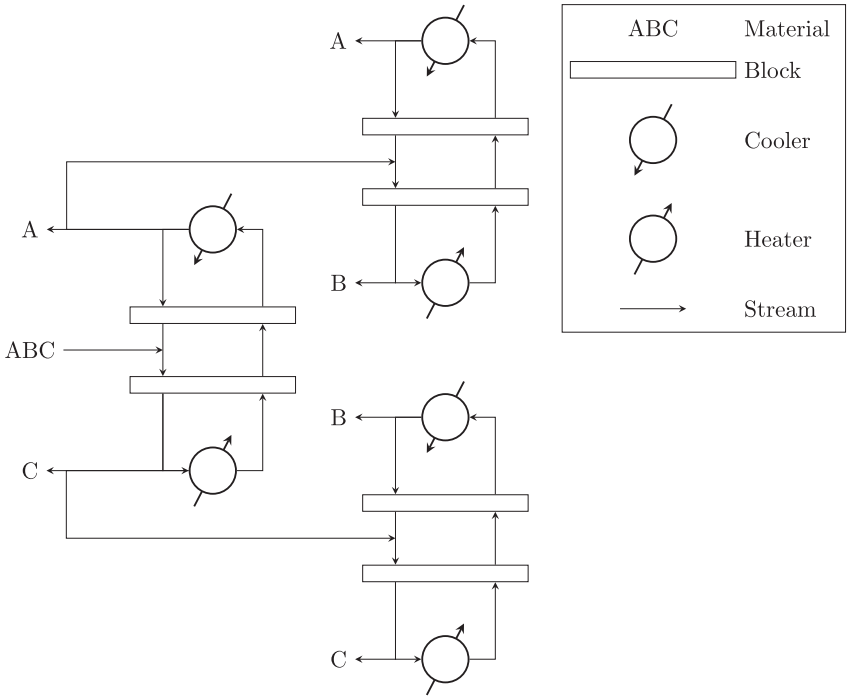

Fig. 7. GMF superstructure for a 3 component sharp split distillation sequence.

Farkas et al. (2005b) address superstructure multiplicity by proposing techniques to consider only R-graphs that are non-isomorphic. They then introduce the "basic" GDP (BGDP) model in the spirit of the GDP formulation in Yeomans and Grossmann (1999), but exploiting the R-graph to avoid introducing additional logical relations that would be required to define certain substructures. Kocis and Grossmann (1988) and Szitkai et al. (2002) perform a computational analysis on literature synthesis problems, demonstrating the procedures to build the BGDP and various mathematical representations (Farkas et al., 2005c). The methodology is then applied to distillation column design and optimization by Farkas et al. (2005a).

As with the P-graph approach, the R-graph exploits mathematical properties of graphs to improve solution strategy performance. Here, the R-graph also takes advantage of logical representability benefits conferred by GDP modeling. However, no software tools exist to support the R-graph approach, and the modern-day benefits of BGDP over a traditional GDP are an open question given the prevalence of linear preprocessing for logical relations.

2.6. Generalized modular framework representation

The generalized modular framework (GMF) representation was introduced by Papalexandri and Pistikopoulos (1996) to simplify

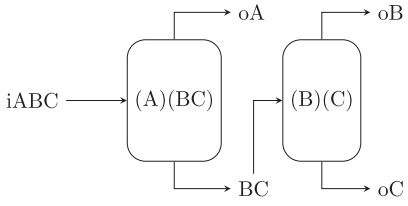

Fig. 8. Group contribution based flowsheet for 3 component sharp split distillation sequence.

superstructure generation with an aim to identify advantageous structural alternatives without needing to explicitly pre-postulate them, much like the state-space representation. GMF was also first developed with a focus on mass and heat exchange networks, with a later distillation sequencing example by Proios et al. (2005) (see Fig. 7). GMF is one of the first major representations to explicitly facilitate design of reactive separation systems (Papalexandri and Pistikopoulos, 1996). The reaction-separation superstructure introduced by Linke and Kokossis (2003) can be seen as a extension based around similar ideas. More recently, GMF has also been extended to explore operability issues of design (Tian et al., 2018b).

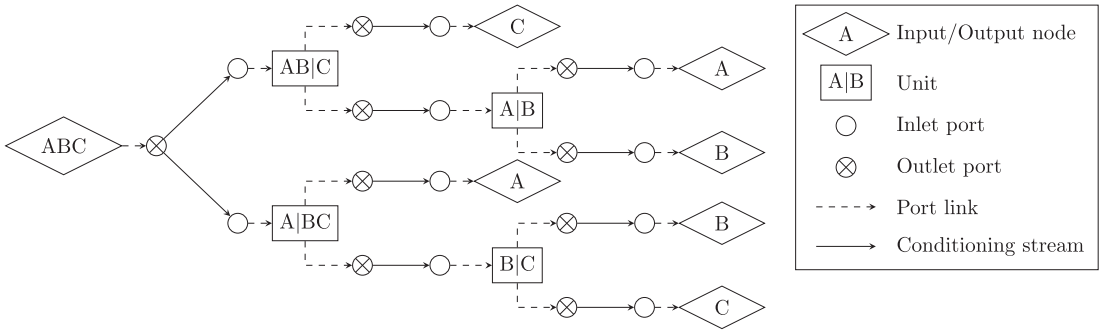

Fig. 9. UPCS representation for a 3 component sharp split distillation sequence.

2.7. Group contribution based methodology

The group contribution based process flowsheet synthesis approach (see Fig. 8) is detailed by d'Anterroches and Gani (2004, 2005), drawing inspiration from group contribution methods in thermodynamic property prediction for molecular design (Fredenslund, 2012). In property prediction, a function is developed relating the contribution of different molecular groups (atoms with different bonding relationships) to the value of a physical property of interest. For molecular design, this prediction function is used to determine the optimal molecular groups that constitute a potentially novel molecule. Applied to flowsheet synthesis, a group can be represented by a process unit or a set of units, with the goal to determine which collection of process units contribute to give the best flowsheet performance. The approach, computer-aided flowsheet design (CAFD), is illustrated for the design of a distillation column by d'Anterroches and Gani (2005).

As with molecular design, a difficulty of this method is obtaining parameters for the prediction function that determines the contribution of various potential process groups to an overall design objective, and their ability to satisfy process specifications. However, if parameters are found that give accurate predictions, evaluation of different process alternatives is generally computationally inexpensive. Tula et al. (2014, 2015) present a recent overview of the CAFD framework.

2.8. Phenomena-building block approach

In the early 2010s, renewed interest in process integration and nontraditional process units led to the development of the phenomena-building block (PBB) approach by Lutze et al. (2013), extending phenomena-centric ideas promoted by Hauan and Lien (1998). As with earlier strategies like the state-space and GMF representations, PBB allows for a broader design space that can automatically generate processes with novel combinations of chemical and physical phenomena taking place within process units. A major challenge with approaches that attempt to propose novel equipment is the selection of an appropriate optimization objective function. As a proxy, many methods use thermodynamic insights, seeking to minimize either energy or exergy use in the process. Kuhlmann and Skiborowski (2016) propose use of development of an PBB equipment database as one solution to this challenge. Other strategies avoid this problem entirely by proposing screening rules that leave a tractable set of promising candidate flowsheets to evaluate (Holtbruegge et al., 2014). However, these screening rules may require simplifying assumptions about the process to be made, and may prematurely exclude advantageous process structures.

2.9. Unit, port, conditioning stream representation

The unit, port, conditioning stream (UPCS) representation (see Fig. 9) was introduced by Wu et al. (2016), consisting of three elements: (a) units, which can be general process units, source units, or sink units; (b) ports, which correspond to unit inlets and outlets, and serve as multi-stream mixers and splitters; and (c) conditioning streams, which link outlet and inlet ports, while also handling temperature and pressure change operations.

The UPCS representation is heavily influenced by ideas in the STN, the P-graph, the R-graph, and the more recent unit operation-port-state (UOPSS) superstructure (Zyngier and Kelly, 2012). The UPCS thus continues the tradition of drawing inspiration from the process scheduling literature (Kelly, 2004; 2005).

As in the P-graph method, Wu et al. (2016) describe an algorithm to generate a UPCS superstructure. First, the set of considered process units are selected based on knowledge of the applicable reaction and separation tasks. Next, inlet and outlet ports are defined for each unit, and streams are created to connect each outlet port to all inlet ports. From this fully-connected starting point, the authors describe four rules to prune invalid and unnecessary connections, based on the set of "minimal" and "feasible" components for each port. Minimal components are those that must be present at an inlet or outlet port. For example, a reactor $A + B \rightarrow C$ would be ineffective without components A or B, so those would be considered minimal components for the reactor inlet port. Feasible components are those that may be present at a given port. All minimal components are also feasible, but a reactor inert I may be considered feasible but not minimal.

Rule 1. All minimal components for outlet ports should be feasible for connected inlet ports.

Rule 2. All minimal components for inlet ports should be feasible in at least one connected outlet port.

Rule 3. All outlet ports connected to a reactor inlet port must contain at least one feasible component that is minimal for the reactor inlet.

Rule 4. All minimal components for a separator inlet port must be feasible in connected outlet ports.

Rule 1 ensures that inlet ports do not receive infeasible components from connections to outlet ports. Rule 2 ensures that each inlet port receives its necessary components. Rule 3 reduces the number of streams connected to a reactor inlet. It is worth noting that in some systems, inerts may be important to the reaction controllability, so care should be given to which components are deemed feasible versus minimal. Rule 4 avoids unnecessary mixing and separation by preventing, among other possibilities, a pure component at a separator outlet from being immediately remixed into the separator inlet.

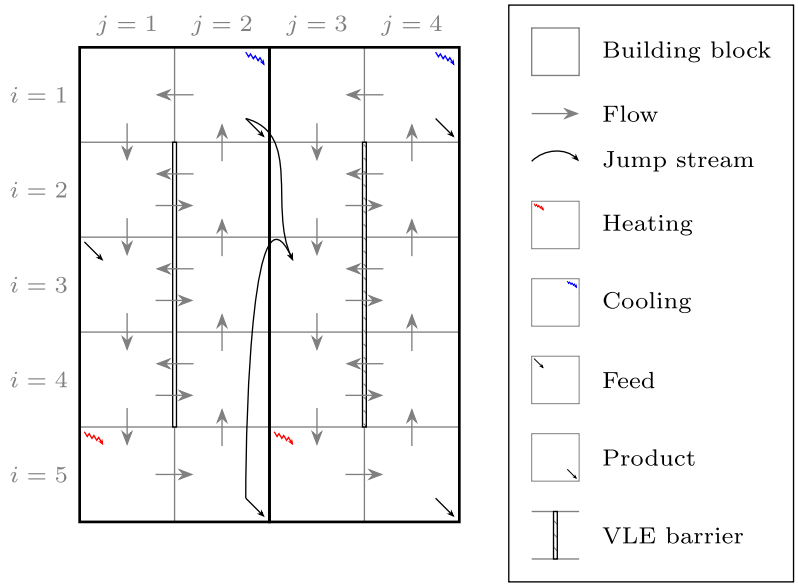

Fig. 10. Building block-based superstructure for a 3 component sharp split distillation sequence.

By shifting temperature and pressure change complexity to the streams, UPCS generates visually simpler superstructures than the STN-OTOE. Use of ports also reduces bypass redundancy, as with the R-graph representation. However, even after screening with the described connectivity rules, automated superstructure generation techniques often produce many more interconnections than are active in the final solution. As a result, the authors also introduce simplification strategies that reduce the number of conditioning streams that must be considered. These simplifications are made based on engineering judgement and restrict the generality of the strategy. However, they reflect real optimization tradeoffs between the generality of a superstructure representation, the fidelity of the physical property calculations, and the computational tractability of its solution. By distinguishing between minimal and feasible components, the UPCS provides more chemical engineering nuance than the P-graph, while also providing a general algorithm for generating its representation.

2.10. Building block-based superstructure

The building block-based superstructure (BBS) (Demirel et al., 2017) is the most recent contribution that attempts to provide a very general representation, capable of capturing aspects of novel equipment design. The representation consists of a two-dimensional grid of blocks, pictured in Fig. 10. Each block represents a control volume, capable of admitting flow across its boundaries to/from its adjacent blocks. Flow across these boundaries can be fully restricted, semi-restricted (to represent membrane/separation systems), or fully open. Each block admits raw material feed into and product withdrawal from the control volume, as well as chemical reactions. Each block also admits temperature and pressure change operations. The control volume of each block is assumed to be well-mixed, with uniform composition, temperature, and pressure in its exit streams.

Unlike the graph-based representations, the BBS approach prioritizes generality and graphical accessibility over solution tractability. By allowing a broad range of operations in each grid cell, the BBS permits the representation of diverse equipment designs without the need to explicitly postulate alternatives, including novel combinations of phenomena that may lead to new equipment designs. Moreover, the two-dimensional grid layout facilitates an elegant visualization of the optimal structure. Discretization in the spatial domain for plug flow reactors and membranes can also be represented as a series of linked grid blocks. However, the structure of the BBS creates a difficult mathematical programming problem.

The BBS therefore challenges the state-of-the-art in modeling and solution techniques. To tackle tractability considerations, two main avenues of investigation have arisen: new solution techniques tailored to the block-grid structure and the careful application of problem-specific engineering expertise. Symmetry is a prominent feature of the BBS, due to the versatility of its blocks. Each block in the BBS is identical, except the boundary blocks, which have fewer interconnections. Li et al. (2018) therefore propose symmetry-breaking constraints to reduce the resulting combinatorial redundancy. Iterative strategies that explore partitions of the feasible region in a “frame-by-frame” manner have also been proposed (Li et al., 2018). However, as with most problems, specialized process knowledge can be a much more powerful tool. By carefully applying domain restrictions, e.g. pre-specifying flow directions, block boundaries, raw material/product block identities, reaction blocks, etc., the problem can be made much more tractable. To aid in this, Li et al. (2018) proposes the use of “jump streams” to connect arbitrary blocks with each other, avoiding the need for specifying empty blocks to accomplish the desired connectivity. An example of their use can be seen in Fig. 10, where the distillate and bottoms of the first column are connected to the feed of the second column. Engineering knowledge also plays a role in superstructure generation. In general, it is an open question how many rows and columns should be postulated in the initial superstructure. For the special case of distillation sequence design, the number of BBS rows should correspond to the number of column trays to be considered. In this example, the BBS representation, pre-specified for the three component sharp split distillation sequence design, resembles the SEN variant 1 (see Fig. 4a). However, successive restrictions of the design space based on engineering knowledge can compromise solution novelty—a central feature of the BBS representation—and so these restrictions should be approached carefully. Ultimately, the BBS provides an initial starting point for approaching the central tradeoff in superstructure-based synthesis (between generality, model fidelity, and tractability) that emphasizes the former two factors, and the solution strategy should be tailored accordingly.

3. Modeling and solution strategies

This paper is focused primarily on discussing different superstructures, but we will briefly touch on the modeling and solution strategies here, because they can often be a factor in selection of the representation. The classic approach involves posing a mathematical programming formulation as a large-scale mixed-integer nonlinear programming (MINLP) problem (Grossmann et al., 2000). Discrete decision variables capture structural alternatives; continuous variables, the process conditions (e.g. temperatures, flowrates, pressures, and equipment sizes). This formulation, expressed within an algebraic modeling platform, would then be sent to a numerical solver to obtain optimal values of the decision variables.

In general, process design is a computationally difficult problem, with nonconvex functions involved describing the process units and their interconnections. These complications can lead to intractable formulations, which modelers often address by imposing simplifying assumptions (e.g. ideal thermodynamics and linear approximations) or tailored restrictions of the search space. Grossmann and Santibanez (1980) address the use of linear approximations in superstructure optimization problems. In addition, more general advanced strategies have been developed to effectively model and solve this difficult class of problems. In the following subsections, we present several themes common among these strategies: logic-based modeling, surrogate models, and decomposition algorithms.

3.1. Logic-based modeling

Process design problems offer significant mathematical structure in the discrete domain, a feature exploited by the graph-based superstructures (P-graph, R-graph, UPCS). Likewise, the structural relationships described by a superstructure can be encoded through logic-based modeling. Generalized Disjunctive Programming (GDP) (Raman and Grossmann, 1994) offers an intuitive way to express the logical-OR (disjunctive) relationship between different process alternatives, while also capturing the connection between these logical clauses and the algebraic relations that describe each respective alternative (Chen and Grossmann, 2019). GDP also allows imposition of logical statements; for example, that selection of a cheaper reactor necessitates feed pretreatment.

GDP is an extension of disjunctive programming from the operations research community (Balas, 2018) to allow for nonlinear algebraic relationships. Therefore, it unlocks a suite of solution strategies that may be applied to the synthesis problem, including systematic reformulations to different MINLP representations that may yield improved computational performance (Trespalacios and Grossmann, 2014). GDP modeling also preserves logical structure for tailored decomposition algorithms (see Section 3.3).

3.2. Surrogate models

In process design, many process unit alternatives may feature complex first-principle models describing transport, thermodynamic, and/or kinetic relationships that are relevant to the problem, but too computationally expensive to include directly in the optimization formulation. In this case, surrogate models (or metamodels) pay a key role—replacing these expensive models with a more tractable approximation that is trained with simulated data from the model, or with experimental measurements (Cozad et al., 2014). Standard optimization algorithms can then be applied using the surrogate models, as in Mencarelli et al. (2019), or trust region-based methods can be used (Eason and Biegler, 2016). If the surrogate does not provide derivative information, then derivative-free "black box" algorithms may be necessary (Rios and Sahinidis, 2013).

Different classes of surrogates can be used, ranging from linear surrogates to Gaussian processes to artificial neural networks (ANNs). In Super-O, piecewise linear representations of different process segments can be used as the building blocks of a superstructure optimization (Bertran et al., 2016). Henao and Maravelias (2010, 2011) introduce a surrogate-based superstructure framework based on the STN-OTOE approach. Fahmi and Cremaschi (2012) integrate GDP and ANNs—the trained ANN surrogates are substituted in place of the first-principle models in a GDP formulation. Kriging interpolators have also been used (Davis and Ierapetritou, 2015; Caballero and Grossmann, 2008). Recently, Schweidtmann and Mitsos (2019) introduced a framework for global optimization of superstructure synthesis problems with ANNs.

Note that in this work, we do not touch on training and parameter estimation concerns associated with using surrogate models. Instead, we refer the reader to a recent review paper in the area of surrogate modeling for process design (McBride and Sundmacher, 2019).

3.3. Decomposition algorithms

Decomposition algorithms that partition a problem into multiple tractable subproblems are commonly used to tackle large-scale optimization challenges. Classic examples of this include the Outer Approximation (OA) (Duran and Grossmann, 1986a) and Generalized Benders Decomposition (GBD) (Geoffrion, 1972) algorithms, which separate the design problem into a master problem that solves a linear approximation of the full space problem and a subproblem that evaluates a fixed flowsheet configuration taking into account the nonlinear relationships. At each iteration, the solution of the master problem proposes a new realization of the discrete variables for the subproblem, and the nonlinear subproblem solution, if feasible, gives new candidate solution points. The subproblem solution also gives new variable values at which to add linearizations to augment the master problem; OA and GBD differ in the generation of these linearizations. Termination occurs when the solution of the master problem converges with the solution of the subproblem.

This two-level decomposition between discrete flowsheet selection and detailed evaluation remains the most common theme among decomposition strategies for process design. Kocis and Grossmann (1989) present a specialized MINLP decomposition approach for synthesis based on Lagrangean decomposition. The discrete elements of an MINLP for process synthesis usually describe logical relationships between superstructure alternatives. With GDP, decomposition may be applied directly on this logical layer. The logic-based outer approximation (LOA) algorithm (Türkay and Grossmann, 1996) exploits this structure to solve the nonlinear subproblems in reduced space, avoiding zero-flow numerical challenges present in MINLP formulations. Logic-based branch and bound (LBB) (Lee and Grossmann, 2000) does the same to solve node relaxations in reduced space, as with the ABB strategy for P-graph (Friedler et al., 1996).

Note that strategies presented in this section differ from hierarchical decomposition (Douglas, 1985) in that the decomposition takes place within an computational solution framework with mathematical guarantees on convergence to optimality. In particular, LBB and a global optimization extension to LOA, GLOA (Lee and Grossmann, 2001), offer convergence guarantees to within an ϵ tolerance. The other discussed decomposition strategies assume convexity, yielding a numerical heuristic for nonconvex chemical process flowsheet problems. Hybrid strategies have also been proposed in which physical insights are used as rules of thumb to screen the solution space before applying a mathematical programming algorithm (Bommareddy et al., 2011).

4. Software implementations

Well-established commercial software tools exist for process simulation, but not yet for process synthesis (Tula et al., 2018). As a result, standard industrial practice for synthesis remains either trial-and-error using simulators, guided by engineering intuition or an expert system package, or the development of special purpose implementations in algebraic modeling systems. However, to provide general capabilities for systematic superstructure synthesis, new tool sets are needed.

To be successful, our community needs software tools to accommodate two classes of users: general users who wish to tackle an understood problem, and advanced users whose design challenges lead them to push the state-of-the-art. The former desire a tool with an accessible interface that will consistently deliver reliable answers for their analyses. The latter, frequently academics or researchers at national labs and major corporations, demand all of the above in addition to the ability to adapt or extend the tool for unknown or unforeseen challenges. The needs of general users limits technology transfer from academia into industry. Academic software rarely benefits from the funding required to create an elegant user interface. Moreover, the finesse required to reproduce academic results often necessitates hiring a student from the relevant research group. On the other hand, without investing in advanced functionality and flexibility for advanced users, innovation in the tool will eventually stagnate, and these users may opt to develop a more capable alternative. Developers must balance these issues among other considerations when choosing where to devote limited resources.

Actively developed synthesis software packages include ProCAFD (Tula et al., 2017), P-Graph Studio (Friedler et al., 2019), MIPSYN (Kravanja and Grossmann, 1990), SYNOPSIS (Tian et al., 2018b), and Pyosyn (Chen et al., 2019), all of which find their roots in academia. ProCAFD is the most sophisticated of these tools in its support of general users, with a graphical user interface and the ability to automatically generate process alternatives from a set of raw materials, products, and reactions. It builds upon pre-existing work in the ICAS (Gani et al., 1997) tool set. P-Graph Studio also features a graphical interface; however, it is less adapted to chemical engineering use, requiring more user input to set up the problem. MIPSYN, on the other hand, has a simple graphical interface, but includes a notion of chemical engineering unit models to aid the user. MIPSYN poses synthesis problems as MINLP or reformulations of GDP models (Ropotar and Kravanja, 2009), which are solved via an integration with the GAMS algebraic modeling platform (Brook et al., 1988). SYNOPSIS and Pyosyn are both newer synthesis frameworks, created as part of two Department of Energy projects: RAPID (Bielenberg and Palou-Rivera, 2019) and IDAES (Miller et al., 2018), respectively. SYNOPSIS is built upon the GMF superstructure representation, though the tool itself has not yet been publicly released. As with MIPSYN, an integration with GAMS allows solution of the resulting MINLP models. Pyosyn, on the other hand, does not prescribe a choice of superstructure, instead focusing on support for high level modeling representations and solution strategies. Pyosyn supports GDP modeling with the open-source Pyomo.GDP (Chen et al., 2018) library, which also enables a suite of solution schemes (Chen and Grossmann, 2019). Specialized chemical engineering support is provided by the IDAES unit model library (Lee et al., 2018), with network representation capabilities using Pyomo.Network.

Most of the described tools have a closed-source code base, with some providing free academic licenses upon request. This has the advantage of protecting intellectual property and generating a revenue stream to fund continued research, general user-oriented features such as improved graphical interfaces, and customer support. However, the community must also support open platforms that allow for prototyping of new innovations and integration of these tools with existing capabilities; otherwise, it risks stagnation as in the process simulation domain.

5. Superstructure-free approaches

Given the challenges of properly generating and solving the superstructure synthesis problem, evolutionary "superstructure-free" approaches have been a longstanding fixture of chemical engineering practice (Nishida et al., 1981). Boonstra et al. (2016) discuss the distinction between superstructure-based and superstructure-free approaches. Superstructure-free approaches also tend to adopt a two-level decomposition approach, separating the discrete topological decision and the detailed flowsheet evaluation, as detailed in Section 3.3. However, instead of a mathematical programming approach to propose flowsheets from the combinatorial search space, an evolutionary algorithm dynamically generates alternative structures, which are then evaluated by an optimization algorithm. Preuss et al., 2014 compare use of an evolutionary algorithm for the upper level and a purely MILP-based approach.

Voll et al., 2012 describe a two-phase hybrid procedure, combining an evolutionary algorithm and a deterministic optimization phase for the energy supply system problem. Neveux (2018) present a similar approach: a structure is generated according to the following mutation rules: (i) block addition between two existing blocks, (ii) block removal, and (iii) permutation of two streams. An NLP is then solved to evaluate the performance of the structure generated. Machine learning has also been proposed as a flowsheet identification technique (Zhang et al., 2019).

Superstructure-free approaches avoid the need for integer variables to model the on/off state of a unit. This often expedites the rate at which new candidate flowsheets are generated. However, rigorous lower-bounding guarantees to assert mathematical optimality without exhaustive enumeration are lost. In applications for which these mathematical lower bounds are unimportant or outweighed by other considerations, superstructure-free approaches can be a valuable search heuristic.

6. Conclusions

Process design is a central challenge of chemical engineering, for which superstructure optimization is a powerful analysis tool. When selecting the correct superstructure representation for a given design problem, the relevant factors are generality, ease of use, and tractability. The representation must capture the relevant choices in processing unit or phenomenological alternatives, clearly represent the space of options, and support formulation of a mathematical programming problem that is amenable to available optimization strategies. In this review, we present the main contributions that led to development of the existing representations, and offer the reader our perspective on their relative strengths with respect to different criteria. We discuss algorithms that exist for automated generation of both the process alternatives as well as their superstructure representation. We also discuss implications that a choice of representation can have on the modeling and solution phases of superstructure-based synthesis.

Finally, we highlight the central tradeoff that exists in tackling superstructure optimization problems: between the generality of the representation, the fidelity of the process unit/phenomena models, and the tractability of solution strategies. The systematic and integrated analysis of alternative structures is the key advantage of the superstructure-based approaches; however, they often yield large-scale non-convex mathematical programming formulations, which are difficult to solve. We highlight various modeling and optimization strategies that aim to overcome this chal-

Table 1
Acronyms.

Acronyms (alphabetical order)	
ANN	Artificial neural network
BGDP	Basic generalized disjunctive problem
CAFD	Computer aided flowsheet design
CAMD	Computer aided molecular design
GDP	Generalized disjunctive programming
GMF	Generalized modular framework
MINLP	Mixed integer nonlinear programming
NLP	Nonlinear problem
OTOE	One task-one equipment
PBB	Phenomena building blocks
PSE	Process system engineering
SEN	State equipment network
SSR	State-space representation
STN	State-task network
UOPSS	Unit-operation-port-state superstructure
UOSS	Unit-operation-stock superstructure
UPCS	Unit, port, conditioning stream
VTE	Variable task-equipment

lenge. In some cases, authors have chosen to pursue evolutionary "superstructure-free" approaches in which alternative process structures are dynamically generated and evaluated from a base case flowsheet. This may lead to faster search speeds in the discrete design space, at the expense of losing finite time mathematical convergence guarantees.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Superstructure synthesis case studies

Table A.2 summarizes literature case studies that have been examined with each representation. We denote with "⋆" those examples involving solution of an MINLP or nonlinear GDP, "•" those involving solution of an MILP (including linear approximation of an MINLP), and "–" where the problem was solved by other means.

Table A.2
Superstructure design examples and case studies.

STN	• Pierce and Realff (1996): multi-chip module scheduling and design ⋆ Caballero and Grossmann (2001): 5 hydrocarbon distillation sequence – Tao et al. (2003): azeotropic separation design ⋆ Ahadi-Oskui et al. (2006): cogeneration power plant, 32 alternatives – Montolio-Rodriguez et al. (2007): acetic acid production ⋆ Karuppiah et al. (2008): corn-based ethanol plant synthesis ⋆ Drobež et al. (2009): biogas process design ⋆ Henao and Maravelias (2011): plant subsystems using surrogate models (amine scrubbing, malic anhydride) ⋆ Martín and Grossmann (2013): biorefinery optimization ⋆ Wang et al. (2014): thermal power plant design
P-Graph	– Halim and Srinivasan (2006): waste minimization • Liu et al. (2006): process retrofit downstream bioprocessing • Voll et al., 2013: distributed energy system design (linearized MINLP) • Vance et al. (2013): sustainable energy supply chain, 21 structures • Heckl et al. (2015): multi-period design for corn processing • Ong et al. (2017): biorefinery design (linearized MINLP) • Edeleva and Stennikov (2018): energy systems optimization • How et al. (2018): biomass supply chain network design • Aviso and Tan (2018): polygeneration • Éles et al. (2018): plant energy supply • Chin et al. (2019): heat-integrated water network (linearized NLP) • Bartos and Bertok (2019): production line balancing – Xu et al. (2015): downstream bioprocess design • Several other examples exist with a similar modeling and solution approach: automotive ammonia production, biomass networks, benzaldehyde production, carbon capture storage, reaction pathway identification, enterprise wide supply, steam supply, and heat integration. We refer interested readers to the recent review paper of Friedler et al. (2019).
SEN	⋆ Smith and Pantelides (1995): ethylbenzene production – Dünnebier and Pantelides (1999): thermally linked distillation columns – Linke and Kokossis (2007): extension for Denbigh reaction systems ⋆ Nie et al. (2012): scheduling and dynamic optimization of batch processes ⋆ Moreno-Benito et al. (2016): batch process development with dynamics ⋆ Cui et al. (2017): coal-based methanol distillation sequence • Madenoor Ramapriya et al. (2018): biorefinery design
State-Space	• Bagajewicz et al. (2002): water treatment network, 8 process units ⋆ Dong et al. (2008): integrated heat and water network design, 3 process units ⋆ Liao et al. (2010): hydrogen distribution network retrofit, moderate size ⋆ Zhou et al. (2012b): water allocation with heat integration ⋆ Zhou et al. (2012a): hydrogen distribution network design for hydrotreating ⋆ Saif and Elkamel (2013): membrane network design ⋆ Hong et al. (2016): heat-integrated water network, 15 process units – Pichardo and Manousiouthakis (2017): hydrogen production from natural gas ⋆ Böcking et al. (2019): membrane network design with experimental validation
R-graph	• Emhamed et al. (2007): desalination facility location
GMF	⋆ Proios et al. (2005): 4 component heat-integrated distillation sequence design ⋆ Algusane et al. (2006): reactive adsorption column design ⋆ Damartzis et al. (2016): amine-based CO2 capture process design ⋆ Tian et al. (2018c): heat exchanger network synthesis with safety and operability ⋆ Tian et al. (2020): methyl tert-butyl ether (MTBE) reactive distillation

(continued on next page)

Table A.2 (*continued*)

Process Group	– Tula et al. (2015): hydrodealkylation of toluene – Lucay et al. (2015): mineral concentration
PBB	* Kuhlmann and Skiborowski (2017): ethanol dehydration – Kuhlmann et al. (2018): transesterification of propylene carbonate – Garg et al. (2019): bio-succinic acid production * Kuhlmann et al. (2019): ethyl tert-butyl ether (ETBE) production
UPCS	* Wu et al. (2017): bio-process design (25 binaries) * Fasahati et al. (2019): cyanobacteria biorefinery * Peng et al. (2019): concentrated solar power plant design * Ng et al. (2019): lignocellulosic biorefinery design • Matsunami et al. (2020): solid drug manufacturing
Building Block	* Li et al. (2018): process integration * Li et al. (2018): fuel gas network synthesis–4 headers, 5 sinks

The references in the table below are curated from the list of articles citing each representation's source publication, as identified by their respective publishers. See Table 1 for definition of acronyms.

Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2020.106808.

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