Recent developments and challenges in optimization-based process synthesis

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Abstract

This paper first reviews recent developments in process synthesis and discusses some of the major challenges in the theory and practice in this area. Next, the paper reviews key concepts in optimization-based conceptual design, namely superstructure representations, multi-level models, optimization methods, and modeling environments. A brief review of the synthesis of major subsystems and flowsheets is presented. Finally, the paper closes with a critical assessment and future research challenges for the process synthesis area.

Introduction

Process synthesis is the assembly and interconnection of units into a process network—involving different physical and chemical phenomena to transform raw material and energy inputs into desired outputs—with the goal of optimizing either economic, environmental, and/or social objectives. The past few decades have seen great advances in process synthesis tools and techniques. Recent theoretical contributions in modeling and optimization offer both new directions and opportunities to address challenges related to environmental initiatives, new energy sources, and industry shifts, as well as the ever-present competitive pressures of globalization. Broad retrospectives on conceptual process design can be found in (1–3) and a recent review in (4). In this work, we aim to review the state-of-the-art in optimization-based process design, reviewing ideas and concepts presented in (5). First, we discuss major approaches to process synthesis, recent developments in the field, and current challenges for conceptual design. Next, we give brief reviews for core areas of optimization-based design. We follow this with a critical assessment of the state-of-the-art, and finally, we discuss future challenges for the field. This paper does not address batch process and scheduling problems; the interested reader is referred to (6–8).

Major approaches to synthesis

The first synthesis techniques were evolutionary in nature (9), whereby heuristics and engineering judgement are used on an existing flowsheet to propose enhancements by adding or modifying process units one at a time. This strategy limits exploration to a neighborhood of the base case. Two classes of approaches emerged to address this limitation: decomposition-based methods (10, 11) and optimization-based methods (5, 12, 13). Decomposition techniques allow for good initial flowsheets, but they have limited ability to consider interactions between different decision layers, such as between separation sequencing and heat integration (14). As an alternative, optimization-based strategies rigorously search through a proposed design space for the optimal configuration. Limitations here arise in our ability to define an appropriate search space, select a suitable degree of approximation, and solve the resulting optimization problems.

Optimization-based strategies involve three major steps: 1. postulation of a set of process alternatives represented by a superstructure, 2. its formulation as a mathematical programming model, and 3.

determination of the optimal configuration by solving the model with an optimization algorithm. Since configurations that are not postulated as part of the search space cannot be found, systematic methods for superstructure generation are needed to ensure that a comprehensive yet concise design space is defined. Formulation involves translating the logic and specifications of process alternatives into an algebraic description that is amenable to optimization algorithms. Process synthesis problems typically result in a discrete/continuous mathematical program of the form (MIP):

$$\min Z = f(x, y)$$

$$s.t. \quad h(x, y) = 0 \qquad \text{(MIP)}$$
$$g(x, y) \leq 0$$
$$x \in X, y \in \{0,1\}$$

In (MIP), we minimize the objective function $f(x, y)$ subject to constraints defined by the equalities $h(x, y)$ and inequalities $g(x, y)$. The objective is to minimize cost, environmental impact, or some other preferred performance metric. If maximization (e.g. for profit) is desired, then the negative of the respective (e.g. profit) function can be minimized. The equalities characterize physical relations and system performance (e.g. mass balances or thermodynamics); the inequalities describe process specifications and equipment limits. The continuous variables x correspond to state or design values such as flowrates and temperatures, and the variables y correspond to binary (0 or 1 value) decisions such as the selection or omission of a process unit. Problems involving multiple objectives can also be addressed by casting them as problems with a single objective. For this, the ϵ-constraint method is a common approach (15).

When any of the functions f, g, h are nonlinear, MIP is a Mixed-Integer Non-Linear Program (MINLP); otherwise, it is a Mixed-Integer Linear Program (MILP). In the absence of binary variables y, the problem MIP is a Non-Linear Program (NLP) or, if all functions are linear, a Linear Program (LP). Recently, a new logic-based modeling framework called Generalized Disjunctive Programming (GDP) has also become popular for synthesis problems. It is interconvertible with MINLPs or MILPs. NLP process synthesis problems were first addressed by Sargent & Gaminibandara (12, 13). The extension to include discrete and logical decisions in the form of MINLPs and GDPs was later made by Grossmann and colleagues (16).

Recent developments

Based upon a belief that no new chemical plants would be built in the US, optimization-based process design saw an erosion of interest in the 90's in favor of scheduling and operational issues. Despite this, progress continued across the major process synthesis research areas, with most attention concentrated in the subsystems of heat exchanger and separation networks. Figure 1 illustrates contributions in the major process synthesis areas before the millennium, between 2000 and 2013, and in the past three years. Out of 1270 process synthesis papers in a recent search of the citation database Web of Science (WoS), 40% deal with heat exchanger network synthesis (HENS) and 30% address mass exchange or separation networks (MENS), including distillation. This finding also aligns with recently reported trends for the citation database Scopus (4). In these subsystems, the papers with the highest citation counts are older ones: (17) with 403 for HENS and (18) with 383 for MENS. Other well-established areas such as reactor network synthesis and general flowsheet design have seen steady, albeit more muted, interest over the years. Many of the prominent papers in these areas were also published before the new millennium.

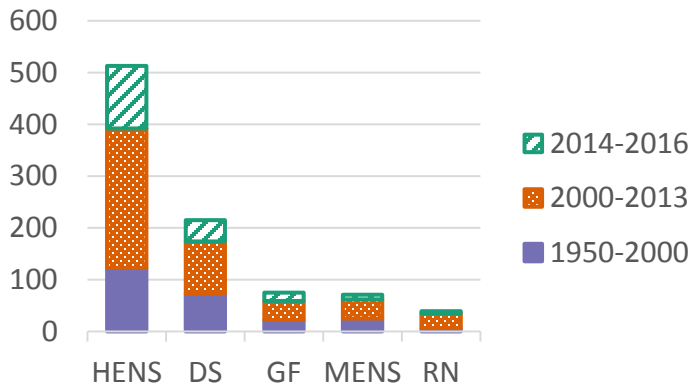


FIGURE 1: WEB OF SCIENCE PROCESS SYNTHESIS CONTRIBUTIONS FROM TRADITIONAL AREAS OF HEAT EXCHANGE NETWORK SYNTHESIS (HENS), DISTILLATION SEQUENCES (DS), GENERAL FLOWSHEETS (GF), MASS EXCHANGE NETWORK SYNTHESIS (MENS), AND REACTOR NETWORKS (RN)

Three major trends drive a recent resurgence in interest for process design: the US shale gas boom (19), a transition in the pharmaceutical industry for Quality by Design (20, 21) and continuous manufacturing (22), and growing environmental initiatives (23). The rising availability of inexpensive shale gas and its liquid natural gases has spurred interest in construction of new chemical facilities and expansion of current ones to exploit the advantaged energy and feedstock sources (24). Similarly, design shifts in the pharmaceutical industry create demand for academic contributions to address the challenges of change in that industry. However, environmental concerns have attracted the most attention, particularly for the design of processes with higher resource efficiency and to accommodate new bio-based feed stocks. These challenges have been addressed by many authors in the literature.

Among newer contributions, there has been particular success in the areas of dividing wall columns, reactive distillation, and water network synthesis. Figure 2 shows the growth in these areas across the past couple of decades. Contributions from Olujic et al. (25) and Stankiewicz (26) have been influential. All results for dividing wall columns and process synthesis have come since 2000, most of which (24 of 39) were published in the past three years. Spurred by recent concerns about freshwater sources, the area of water network synthesis has seen great growth, with 58 of 92 WoS contributions published since 2000, 23 of which were published in the past three years. Multi-objective optimization has also seen growing prominence due to environmental concerns (23, 27). Especially impactful was the introduction of life-cycle analysis (28) at the turn of the century.

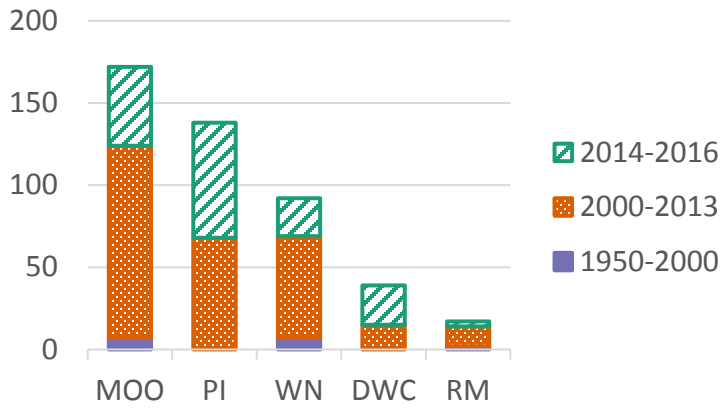


FIGURE 2: WEB OF SCIENCE PROCESS SYNTHESIS CONTRIBUTIONS FROM GROWTH AREAS OF MULTI-OBJECTIVE OPTIMIZATION (MOO), PROCESS INTENSIFICATION (PI), WATER NETWORKS (WN), DIVIDING WALL COLUMNS (DWC) AND RIGOROUS MODELS (RM)

Another area of process design that is transformative by definition (29) is process intensification (PI), which promises orders of magnitude improvements in process characteristics such as reaction rates or equipment volumes through use of increased fields or gradients; modified transport mechanisms, geometries, and driving forces; and integrated equipment (30). Process Systems Engineering (PSE) and PI have complementary goals in seeking process improvements and their coupling is well-suited (31). In fact, under the definition for PI as "any chemical engineering development that leads to a substantially smaller, cleaner, and more energy-efficient technology" (29), most process synthesis activities can be regarded as intensification. The synthesis of intensified processes has been a very popular subject in recent years, with 138 entries in WoS, with more than half of those published within the past three years. A recent review of PI from a process synthesis perspective can be found in (32). High impact contributions in this area include a paper by Cardona & Sanchez on intensified processes for fuel ethanol production (33). Recently, Lutze et al. have also demonstrated a hierarchical decomposition-based synthesis method starting from process phenomena building blocks (34). Intensification promises to be a powerful tool to address environmental challenges (35). Aside from the benefits of efficiency improvements for the environment, PI can be applied to carbon capture processes (36) in order to improve their economics and make them more viable.

Process synthesis also benefits from advancements in solver and computational performance. Continued gains in these areas have made tractable classes of problems that were previously too difficult. Improvements in computing power and memory facilitate solution of larger and more complex problems. Coupled with the development of nonlinear solvers capable of exploiting sparsity, algorithms can solve large-scale NLPs and thus consider rigorous models that more accurately represent the underlying process. Of the citations in WoS for keywords "rigorous model" with "process design/synthesis", all have been since 2000, with the most heavily cited being a reactive moving bed model (37). Significant advances in MILP solvers, including the introduction of cutting planes (38), have made possible the solution of linear and discrete problems with hundreds of thousands of variables and constraints. MINLP and GDP solution techniques have taken great strides as well (39, 40). The growth of global optimization (41) for both nonlinear and discrete problems offers decision-makers mathematical certainty for a given model that the solution found is within a certain tolerance from the best possible

solution. Improved solver performance has also made consideration of multiple objectives (3) and process and parameter uncertainty (42) much more tractable.

There has also been progress made on the theoretical and practical aspects of modeling due to the emergence of GDP (16) and Object-Oriented Modeling (OOM) (43). These complementary developments facilitate structured model creation and provide a systematic framework for expressing the logic of superstructure alternatives using higher-level logical operators and disjunctions, for which automatic reformulations can be applied to yield MILPs or MINLPs of varying complexity. The result for synthesis will be the ability to further standardize the model building process and enable easier error-checking and validation. Detailed descriptions of both GDP and OOM are given in later sections.

Major challenges

Despite progress in the area, challenges remain both in theory and in practice. The ability to robustly solve large, industrially-relevant problems remains limited. Even simple flowsheet structures such as mixers and splitters give rise to non-convex nonlinear expressions in the form of bilinear split fractions and mass balances (44). Incorporation of process thermodynamics and transport phenomena further complicate the ability of optimization algorithms to arrive even at a feasible design, let alone an optimal one. Therefore, finding a good initial starting point for the optimization problem can be a major challenge. One option is to start the optimization with variable values initialized at a feasible base case design obtained by other means. Barttfeld et al. present a thermodynamics-based initialization approach for distillation column design (45). Another promising approach to the initialization challenge was presented by Amundsen & Swaney using a strategy based on a canonical primal-dual formulation that guarantees convergence of a nonlinear model (46, 47), at least for simulation of a specified process configuration. Due to the inherent non-convexities, searching for globally optimal solutions raises another layer of difficulties. Specialized assumptions are typically necessary in order for the problems to be tractable. For example, fixing temperatures to a single value or a discrete set of values can greatly simplify heat balances and thermodynamic calculations. However, these assumptions yield approximations that may not be appropriate for a given process flowsheet. Therefore, there has been no consensus for a unified approach to solving flowsheet problems.

There are also challenges we face in leveraging synthesis and expanding its capabilities to address social and industrial issues. One area of great interest is in process design under uncertainty. During conceptual design, there are often process parameters that are not well known, such as kinetic rate constants or product and feedstock prices. Design under uncertainty allows us to systematically hedge against exceptional realizations of process parameters through a combination of planned recourse actions and/or design tolerance. Initial work in process design under uncertainty involved theoretical advances in flexibility analysis (48, 49). Later, two-stage stochastic programming was used by Pistikopoulos & Ierapetritou (50). A review of these early developments can be found in (51). Other theoretical advancements followed in the late 1990s, both in formulation (52, 53) and solution algorithms (54). With the attention shift towards scheduling and operations, there have been fewer recent contributions in process synthesis with uncertainty. However, there have been a few recent publications in which uncertainty analysis is extended to tackle issues of process sustainability (55–57).

With rising demands on natural resources around the globe, sustainability is likely to feature even more strongly in considerations for conceptual process design. Energy use in developing countries continues to grow at compounding rates (58) and sources of fresh water are increasingly strained. In fact, a water

supply crisis is rated by the World Economic Forum as one of the most likely and consequential of existing global risks (59). Meanwhile, CO_2 emissions have continued to grow even with the stall in industrial investment due to the recent global financial crisis (60). With growing public support for emissions reduction programs, carbon-intensive industries face increasing regulatory risk in their operations.

Process design is well-positioned to help society and industry cope with these challenges. Intelligent green-field and retrofit designs can help minimize resource-intensity of industrial processes so that developing countries can continue seeing growing standards of living while industry transitions towards more sustainable processes. One growth area of sustainable design is incorporation of biomass as a chemical feedstock (61). Due to the renewable fuel standard in the US, large volumes of corn ethanol have been produced (62, 63). However, production of ethanol from crop corn has raised issues of competition with the food supply chain, leading to artificially increased global food prices. Therefore, research is ongoing on processes for non-food sources, such as switchgrass (64–66) and other inputs (67).

Core areas of optimization-based conceptual design

Superstructures

Postulation of a set of alternatives, represented by a superstructure, is the first step in an optimization-based approach to process synthesis. Selection of the appropriate superstructure is important not only because the optimal configuration can only be found if it is described in the superstructure (1, 68), but also due to the modeling implications that it can have. Two commonly used types of representations are the State-Task Network (STN) and State-Equipment Network (SEN).

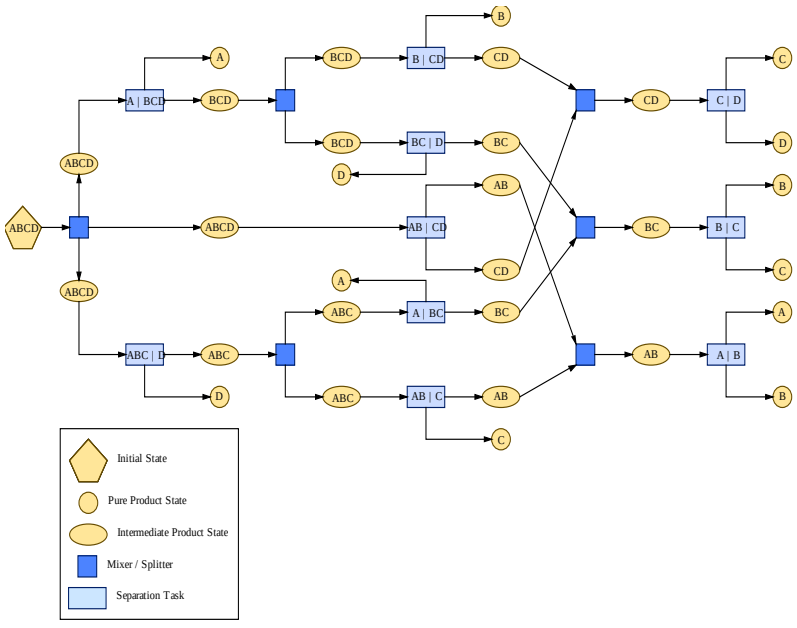
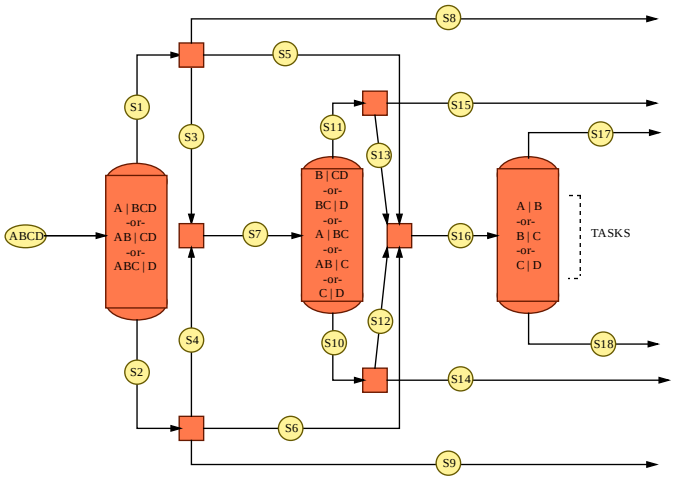


FIGURE 3: STATE-TASK NETWORK (STN) SUPERSTRUCTURE, FIGURE FROM (69)

The STN representation (see Figure 3) is inspired by contributions in scheduling (70) and consists of state nodes connected by distinct processing tasks that transform one state to another. Equipment

assignment is handled implicitly in the model, and can accommodate use of a single piece of equipment for multiple tasks, such as in batch scheduling. The SEN representation (see Figure 4) developed out of a desire to decrease the number of process nodes required to describe a distillation sequence (71). For a four-component system with sharp separations, three process nodes are required to describe all possible configurations with an SEN versus ten for the STN. The SEN is also better suited for use of rigorous distillation models, since only three columns would need to be modeled and none of the columns become inactive, leading to zero-flow singularities. Yeomans & Grossmann give a detailed comparison of these two representations and present the respective GDP models (72).



STATE DEFINITION

S1- A, AB, ABC	S6- CD	S11- B, BC, A, AB, C	S16- AB, BC, CD
S2- BCD, CD, D	S7- BCD, CD, ABC	S12- CD, BC	S17- A, B, C
S3- ABC	S8- A	S13- BC, AB	S18- B, C, D
S4- BCD, CD	S9- D	S14- C, D	
S5- AB	S10- CD, D, BC, C	S15- A, B C	

FIGURE 4: STATE-EQUIPMENT NETWORK (SEN) SUPERSTRUCTURE, FIGURE FROM (72)

The state-space model introduced by Bagajewicz & Manousiouthakis presents a perspective inspired by work in HENS and MENS, where the interconnections of a superstructure are handled in a distribution network and the process operations take place in an operator network (73). Under the state-space framework, a distillation sequence can be represented as interacting sets of heat and mass exchange networks. The result is a linear programming problem when certain process conditions, such as temperatures, are pre-specified. A review of other specialized superstructures developed for subsystems can be found in (72), and they are also discussed later in the subsystems section.

Systematic generation of the superstructure in order to include all relevant alternatives was first discussed by Friedler and colleagues, who presented the concept of a process graph (P-graph) as an extension of graph theory (74) and gave a polynomial time algorithm (75) to determine the necessary interconnections given a set of inputs, processes, and outputs. More recently, Wu et al. present a new representation composed of process units, ports, and conditioning streams, while also giving a set of four rules by which to generate simple superstructures describing feasible processes (76).

Models (high level, shortcut, rigorous)

Following postulation of a superstructure, its nodes and interconnections must be translated into the variables and constraints of a mathematical model. In general, there is not a unique relationship between a model and its underlying superstructure. That is, the same superstructure can be modeled in

different ways—including at various levels of modeling detail. Models can be characterized into three main levels of detail: high-level aggregate models, shortcut models, and detailed rigorous models.

High-level (aggregated) models

The most simplified models are aggregated models, where the synthesis objective is focused only on the dominant elements of the objective or system constraints. These models take a high-level view of the design problem and are appropriate when little detailed process information is available or desired. They are frequently used in the context of targeting in order to provide an idea of the improvement possible when using a more detailed model. Aggregate models include the transshipment model (see Figure 5) for predicting minimum utility or number of exchangers in HENS (77) and MENS (18), distillation models to minimize utility cost (78), and reactor models to maximize yield (79). Since aggregate models tend to focus on one objective and have simpler constraints, they also tend to be optimistic in their predictions versus a more nuanced model, though this is not always true.

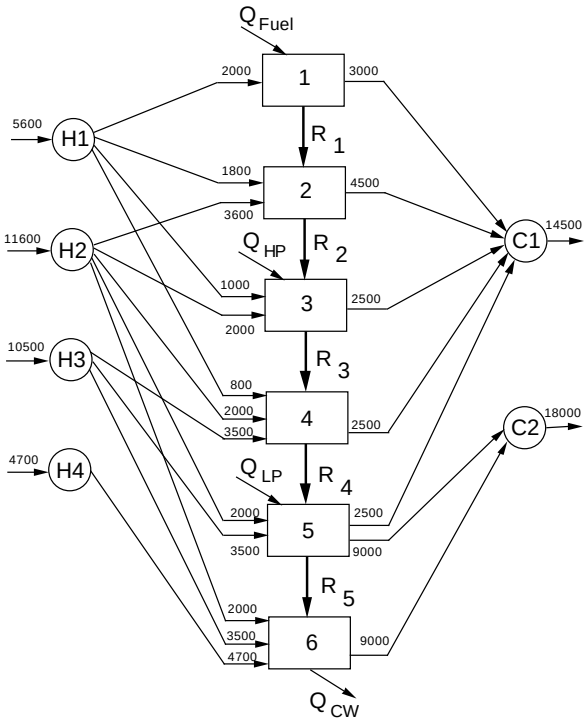


FIGURE 5: TRANSSHIPMENT LINEAR PROGRAMMING MODEL FOR HEAT EXCHANGE NETWORK SYNTHESIS

Shortcut models

At a more detailed level of approximation, shortcut models provide better predictions. These models involve more complex cost functions in the objective, yet retain a simpler nonlinear description of the process units. Shortcut models enable the modeler to predict more accurate profits and costs, including discontinuous investment functions, while maintaining tractability in the overall model. As a result, shortcut models are popular for performing global optimization. However, though simplified constraints are used for the process models, the resulting NLP, MINLP, or GDP is still typically nonconvex due to mass and energy balances on mixing and splitting nodes. Examples of shortcut models can be found for heat exchanger networks (17, 80), distillation sequences (72, 81, 82), and general process flowsheets (76, 83–87).

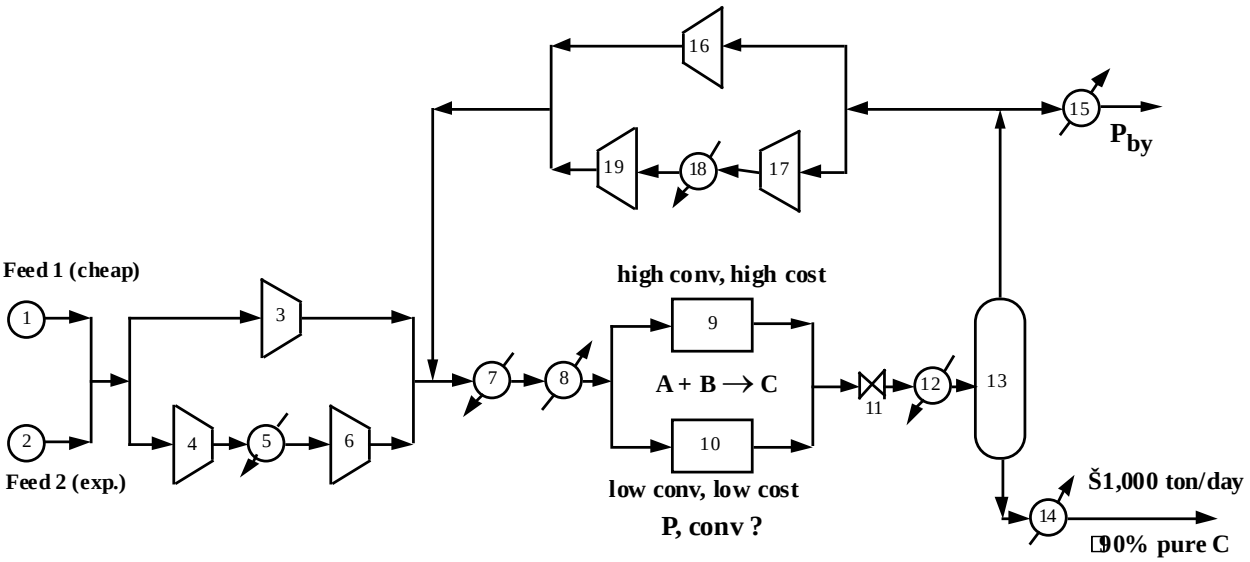


FIGURE 6: SHORTCUT FLOWSHEET SUPERSTRUCTURE, FIGURE FROM (85)

Rigorous models

Rigorous models involve complex unit performance predictions, including equilibrium- or rate-based mass and/or heat transfer. A major barrier in the optimization of these systems is that the models are typically implemented in "black" boxes in which only function evaluations can be performed. Derivatives are typically not available and must be obtained by finite differences, which are subject to numerical inaccuracies. Furthermore, due to the potentially nonconvex equations involved in characterizing the additional process details, there can be local optima for the resulting mathematical program. Moreover, with growing problem size, global optimization methods may become intractable. As a result, finding a good initial starting point for optimization of rigorous models can be a challenge in itself. The bulk of interest in rigorous models has been related to synthesis of distillation sequences (71, 88–92).

Selection of the appropriate level of detail is an important modeling task, driven by the specific engineering needs and modeling intent. The modeler must contend with the tradeoff between solving approximate models exactly, versus solving more exact models only approximately. In general, aggregate models result in smaller LP, NLP, or MILP problems that may solve in seconds to minutes while shortcut models and rigorous models yield larger MINLP (or GDP) problems that require much more computational effort.

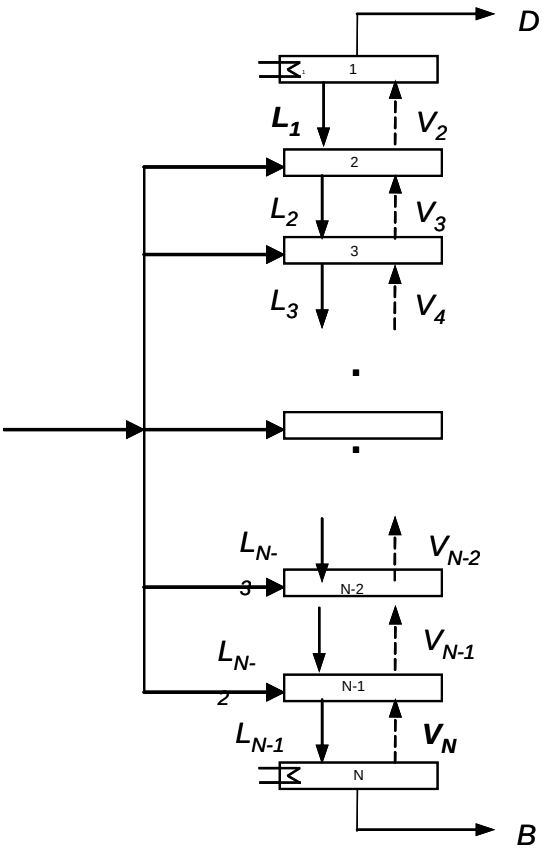


FIGURE 7: RIGOROUS MODEL SUPERSTRUCTURE, FIGURE FROM (93)

GDP

Even after specifying a model detail level, there is no unique way to express the logic encapsulated in the superstructure as a set of variables and constraints. Generalized Disjunctive Programming (GDP) provides a remedy to this by allowing the modeler to formulate discrete/continuous optimization problems using higher-level logic (94). GDP can be seen as an extension of disjunctive programming (95) in which both nonlinearities and discrete variables are introduced into the model. Recent reviews of GDP can be found in (16, 40, 96).

GDP models involve continuous and Boolean variables with constraints in the form of algebraic expressions, conditional constraints encapsulated within disjunctions, and logical propositions. The resulting mathematical program is of the form:

$$\min Z = \sum_{k \in K} c_k + f(x)$$

$$s.t. \quad g(x) \leq 0 \qquad \text{(GDP)}$$

$$\bigvee_{j \in I_k} \begin{bmatrix} Y_{jk} \\ r_{jk}(x) \leq 0 \\ c_k = \gamma_{jk} \end{bmatrix}, \qquad k \in K$$

$$\Omega(Y) = True$$

$$x \in X$$
$$Y_{ki} \in \{True,\ False\} \quad k \in K,\ j \in I_k$$

where x are continuous variables and Y are the Boolean variables. The objective function contains terms c_k corresponding to selection of certain disjunctions as well as a function $f(x)$ on the continuous variables. These two terms typically correspond to fixed and operating costs, respectively. The algebraic constraints $g(x) \leq 0$ represent constraints (inequalities or equalities) that must be satisfied for any realization of the discrete choices, while the constraints $r_{ki}(x) \leq 0$ and fixed charge $c_k = \gamma_{jk}$ only need to be valid in the disjunctions for which the corresponding Boolean variable Y_{jk} is $True$. The logical constraints $\Omega(Y) = True$ then describe the logical propositions relating Boolean variables.

In the context of process synthesis, GDP provides a convenient way to formulate a model for a superstructure (85). The constraints $g(x)$ describe superstructure nodes that are "fixed" or always present in the final design. The disjunctions represent the choice among process alternatives, with the binary variables Y_{jk} denoting the presence or absence of nodes (e.g. tasks or equipment) in the final process configuration. Process constraints related to a node are thus only enforced if the node is selected in a given design. Logical constraints $\Omega(Y)$ dictate relationships among the superstructure nodes. For example, the need to select a better separation unit if the cheaper reactor is chosen can be represented using the logical implication operator: $Y_{\text{cheap reaction}} \Longrightarrow Y_{\text{better separator}}$. Other examples of logical implications can be found in (16). An alternative formulation based upon the ideas of process synthesis can be seen in (GDP').

$$\min Z = \sum_{k \in K} c_k + f(x)$$

$$s.t. \quad g(x) \leq 0 \qquad \text{(GDP')}$$

$$\begin{bmatrix} Y_k \\ r_k(x) \leq 0 \\ c_k = \gamma_k \end{bmatrix} \vee \begin{bmatrix} \neg Y_k \\ B^k x = 0 \\ c_k = 0 \end{bmatrix}, \qquad k \in K$$

$$\Omega(Y) = True$$
$$x \in X$$
$$Y_{ki} \in \{True,\ False\} \quad k \in K$$

Here, the more general disjunction over terms j is replaced by an explicit disjunction between the existence or absence of a node. When the node is present ($Y_k = True$), the corresponding equations are enforced. When it is absent ($\neg Y_k = True$), then linear constraints $B^k x = 0$ force a subset of variables to zero, such as flow rates, while allowing others, like temperature, to vary. The fixed costs c_k for an absent node are also set to zero.

Both (GDP) and (GDP') can either be solved either by reformulation into an MILP/MINLP, followed by traditional MILP/MINLP solution techniques, or by directly addressing the disjunctions via logic-based methods (97). The big-M (BM) and hull reformulations (CH), which consist of the intersection of convex hulls for each disjunction, are the most common alternatives for reformulation of a GDP into an MINLP. The CH technique results in a tighter feasible region than BM (87), but it also results in a large problem size with many more variables and constraints. The resulting performance is thus difficult to ascertain ahead of time (98). Intermediate strategies are also possible, with the BM model augmented by addition of cutting planes (99) or by the use of multiple different big-M parameters (100). These reformulation

techniques allow the modeler to take advantage of advancements in MILP/MINLP solution algorithms. On the other hand, logic-based methods offer their own set of advantages. Two of these specialized algorithms are Logic-based Branch and Bound (101, 102) and Logic-based Outer-Approximation (LOA) (85). LOA is an extension of Outer-Approximation in which NLP subproblems are solved in a reduced space. For a given process configuration proposed by the MILP master problem, the subproblem contains only the constraints present in active disjunctions; all others are disregarded. The result is both improved efficiency and robustness, as zero-flow singularities through inactive process units are avoided. LOA can handle non-convexities through the use of penalty functions and slack variables (93). Alternatively, the extension of LOA for rigorous global optimization is also available (103, 104).

Modeling environments

Various modeling environments are available for the formulation and solution of mathematical programming models. The two most established platforms are GAMS (105) and AMPL (106). These environments typically require models to be input explicitly in algebraic form. These are then automatically translated into inputs through various interfaces to solution algorithms, which return a formatted output file. Of the two, GAMS is very strong in the longevity of backwards support for their syntax. A model written thirty years ago will still run today with few if any modifications. This is all the more impressive given the shifts in the computing world during this timeframe. On the other hand, AMPL has shown greater interoperability, with custom third party programs able to access compatible solvers through the AMPL Solver Library. More recently the modeling platform AIMMS (107) has also grown in popularity, particularly among the industrial community. A book by Kallrath provides a more detailed review of the established modeling systems (108).

The past few years have seen another generation of modeling environments enter the scene with the introduction of PyOMO (109) and JuMP (110). These two modeling frameworks are directly built upon the Python and Julia higher-level programming languages, respectively. This allows the modeler direct access to the modeling objects, facilitating the paradigm shift towards object-oriented modeling and enabling easy prototyping of meta-algorithms.

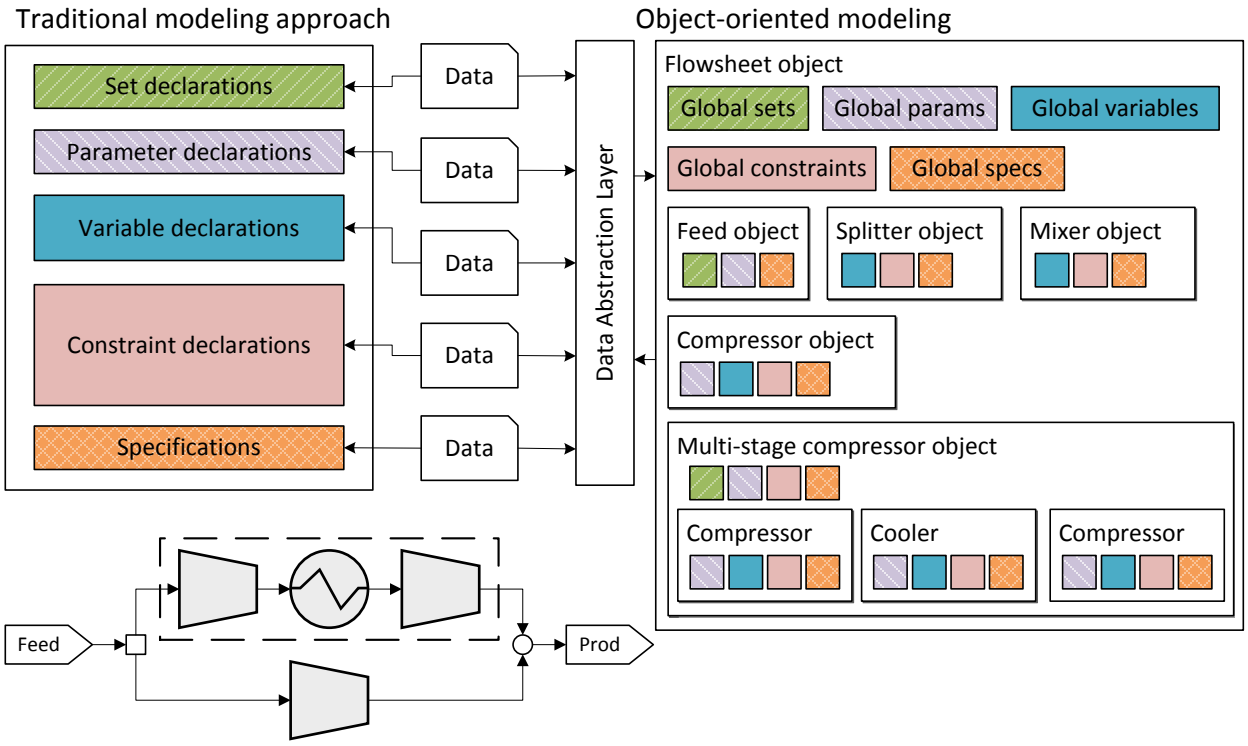


FIGURE 8: CONTRASTING TRADITIONAL AND OBJECT-ORIENTED MODELING APPROACHES

Object-oriented modeling (OOM) provides an intuitive way of modeling superstructures in which variable and constraint definitions for various superstructure elements are encapsulated within respective classes of objects, organized in a hierarchy. The quest for modularity is a long-standing one (83), with recent interest as well (76, 111). The new generation of modeling environments makes this vision possible. In the PyOMO language, Block objects are well-suited for this role (43). For example, a Flowsheet block may contain several equipment blocks, including a Multi-stage Compressor block, which itself would contain multiple Compressor blocks and Cooler blocks as well as linking constraints dictating that shaft work among constituent compressors are equal. OOM is also symbiotic with a GDP approach by placing variables and constraints in intuitive groupings for disjunctions, which can be seen as conditionally active blocks. Furthermore, OOM enables code sharing between common model elements, as material balances for mixer and splitter blocks in various parts of the superstructure are not likely to different greatly. In contrast to the traditional approach, the OOM paradigm produces models that are more readable and easier to validate.

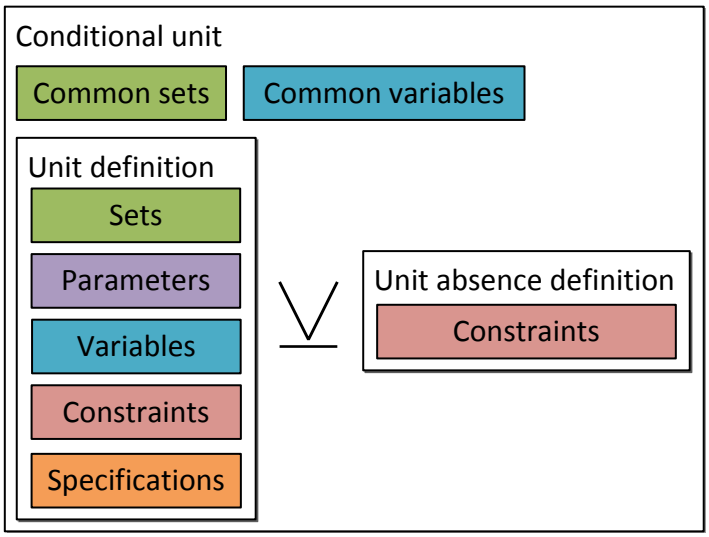


FIGURE 9: USE OF OBJECT-ORIENTED MODELING WITH GENERALIZED DISJUNCTIVE PROGRAMMING

By allowing modelers to perform programmatic manipulations of modeling objects, the newer environments also enable easier prototyping of novel solution algorithms. Programmatically generated cuts can be automatically added to an existing model and different classes of constraints can be deactivated or reactivated as needed within a Python or Julia script to implement algorithms, such logic-based outer-approximation.

Optimization methods

After a model is constructed, the next step is solving it with an appropriate optimization algorithm. Although computational gains through improved processors and especially larger memory capacities have been impressive, algorithmic gains have been even greater (38). Codes for solution of LP problems are by this point very mature, with two main methods: the simplex algorithm (112) and interior point methods (113, 114). A review of advances in linear programming can be found in (115). For MILPs, the classical simplex branch and bound strategy (116) is now augmented by several cutting plane techniques including lift-and-project (117), Gomory mixed-integer (118), and mixed-integer rounding cuts (119). Bixby & Rothberg give an excellent analysis of the computational performance enhancement for each class of cutting planes (38), while a comprehensive overview of the theory can be found in the monograph (120). The most popular solvers for LP and MILP problems are the commercial packages CPLEX (121), Gurobi (122), and XPRESS (123). A review of noncommercial options is available in (124).

Nonlinear programming solvers have traditionally relied either on the successive quadratic programming (SQP) (125–127) or reduced gradient (128) strategies. Excellent descriptions of the underlying theory can be found in textbooks by Fletcher (129) and Bazaraa et al. (130). SQP codes include SNOPT (131), while reduced gradient codes feature CONOPT (132) and MINOS (133). Recently, interior point methods, inspired by work in the LP community, have also become a viable alternative, particularly for large-scale problems. IPOPT (134) and KNITRO (135) are the most common of these. A recent review of these NLP codes and their nuances can be found in (136). Another recent development has been a proliferation in codes for derivative-free optimization (137). These codes allow for optimization of systems in which derivative information is not available, such as in “black box” simulations. In contrast to the breakaway success of linear and mixed-integer solvers, few commercial nonlinear solvers are available—CONOPT is

the main exception—with most code development taking place in academic settings. One reason for this may be due to the customer service implications of robustness for NLPs. While most LPs and MILPs, even poorly formulated, will yield a solution, an NLP poorly formulated or not initialized may fail to converge.

This challenge extends to the case of MINLPs, whose solution relies on use of NLP, MILP, and/or LP sub-problems. Recent reviews of MINLP methods can be found in (5, 40, 138, 139). The main methods for tackling MINLPs include Branch and Bound (B&B) (140), Generalized Benders Decomposition (GBD) (141, 142), and Outer-Approximation (OA) (143). B&B is an extension of the MILP strategy in which sub-problems are NLPs rather than LPs. Both GBD and OA iterate between an MILP master problem that selects new 0-1 variable configurations and NLP sub-problems for fixed values of the 0-1 variables. At each iteration, new cuts are added to the master problem, which predicts lower bounds on the objective value. Sub-problems, if feasible, determine the upper bounds. Termination occurs when the bounds converge. The main difference between GBD and OA lies in the cuts added at each iteration. OA adds linearizations of the nonlinear functions while GBD derives its cuts from Lagrangean functions parametric in 0-1 variables. Other techniques include LP/NLP B&B (144) and α-ECP (145). The main codes available for general convex MINLPs include DICOPT (93), Bonmin (146), α-ECP, FilMINT (147), MINLP_BB (148), and SBB (149).

The methods discussed above for NLPs and MINLPs yield guaranteed convergence to the global optimum only for convex problems. In the presence of complex nonlinearities, rigorous global optimization techniques are necessary to guarantee global optimality. These techniques take advantage of special mathematical structures in the optimization problem, such as bilinear, linear fractional, and concave separable terms, whose combination can express the range of algebraic models excluding trigonometric functions (150). Using the special structures, rigorous convex envelopes can be constructed and iteratively tightened (151–153). A review of global optimization methods can be found in (41). The most popular codes for general purpose global optimization of NLPs and MINLPs include BARON (154), ANTIGONE (155) and SCIP (156), as well as the open source code Couenne (157). While these general purpose solvers are growing more powerful, knowledge of special problem structure can lead to development of specialized codes that may be more robust, converge faster, or enable treatment of larger problem sizes. Examples include outer-approximation algorithms (158) or branch and contract (159). Global optimization algorithms are also available for GDP models (96, 101, 160).

Non-rigorous techniques for global optimization, such as simulated annealing (161), genetic algorithms (162), and Tabu search (163), also continue to be popular in situations when objective function evaluations are cheap and derivative information is not readily available. These methods can provide good heuristic solutions. However, they do not give any guarantee of convergence to a rigorous global solution in finite time, and they tend to depend upon ad-hoc penalty functions for constraint handling.

Subsystems and flowsheets

In the following section, we give a brief overview of advances in model development for subsystems (heat exchanger networks, steam and power, distillation networks, mass exchange and water networks, and reactor networks) and process flowsheets. Where possible, we refer the reader to authoritative reviews on subsystems and focus on the ideas that have had the most impact.

Heat exchanger networks

Heat exchanger network synthesis (HENS) has attracted by far the most interest of the process synthesis subsystems. As a result, many excellent reviews are available in the area. Furman & Sahinidis provide the most highly cited review (164). Morar & Agachi provide a more recent update (165), while Klemes & Kravanja discuss developments in both mathematical programming and pinch-based approaches (166). Much of the attention on HENS is due to interest in heat integration. Beginning with (167, 168), many recent contributions incorporate heat integration as part of a larger process synthesis or optimization problem (169–171). Progress continues to improve the scope and size of tractable problems (172). Computational tools for HENS synthesis include SYNHEAT (17) (see Figure 10) and Aspen Energy Analyzer (173).

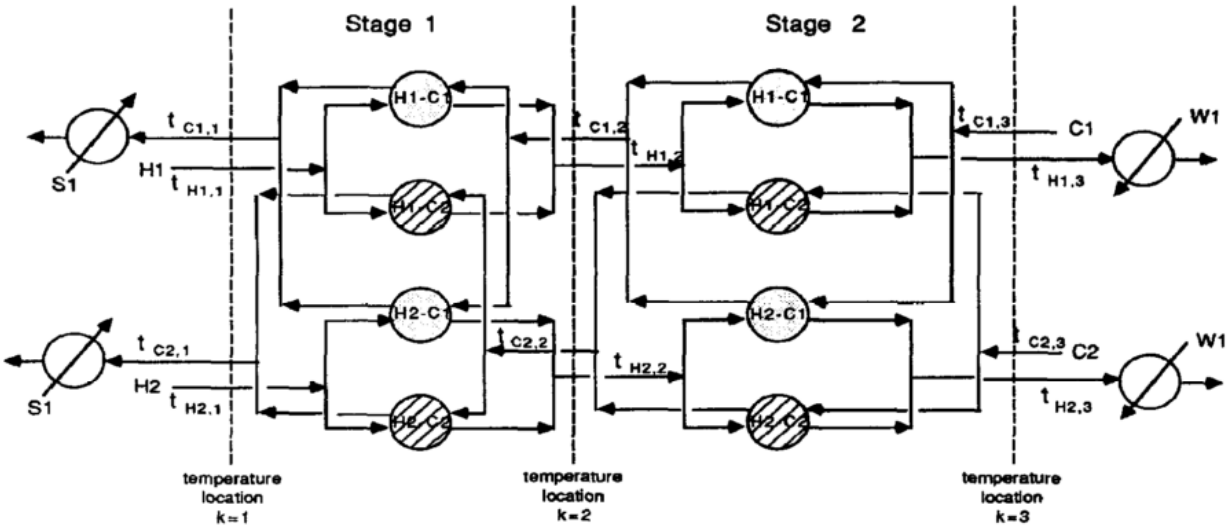


FIGURE 10: HEAT EXCHANGE NETWORK SUPERSTRUCTURE FROM (17)

Steam and power

Steam and power plants provide steam utility to the process and, if needed, electric and mechanical power to the rest of the processing plant. Initial LP models for optimizing utility production were proposed by Petroulas & Reklaitis (174), followed by an MILP formulation by Papoulias & Grossmann (175) for fixed utility demands and operating conditions. Refinements continued in the 1990s (5), including publication of one of the first MINLP models for utility network synthesis (176) (see Figure 11). Towards the new millennium, research attention shifted more towards operational aspects (177). Recent interest in carbon capture for electricity generation and cogeneration has led to newer contributions (170, 178–181). A recent review of utility plant synthesis can be found in (182).

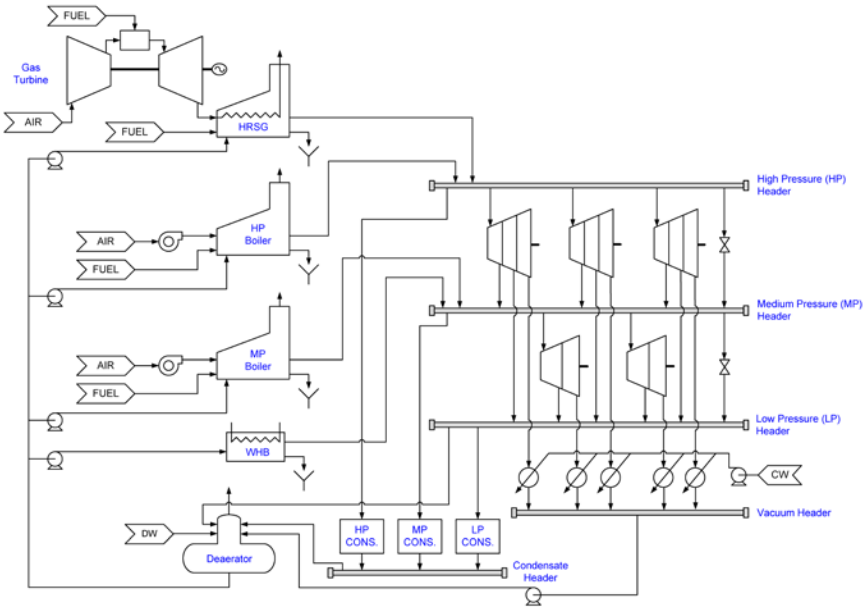


FIGURE 11: UTILITY PLANT SUPERSTRUCTURE, FIGURE FROM (176)

Distillation network synthesis

After HENS, distillation network design has received the most attention due to the importance of separations in the process industry. Distillation is an expensive operation, both in terms of investment and operating costs (183), yet its ubiquity testifies to its effectiveness as a separation method, even for non-ideal and azeotropic mixtures. As a result of its prominence and expense, many contributions have been made to improve its design and operation (184). A review of early techniques can be found in (185, 186). Distillation synthesis includes one of the earliest uses of superstructure optimization (13), giving a tray-by-tray NLP model. A later MILP model opened the way for design of heat integrated distillation sequences (69). With the ability to heat integrate distillation columns, significant operating cost reductions became possible, as not only is the hot utility load on one column reduced, but the cold utility requirement for another column is also reduced. Subsequent modeling contributions enabled treatment of more complex column configurations and cost functions (187–189). The next major development was the introduction of tray-by-tray rigorous models (71, 190, 191), providing a more realistic prediction of column performance. Recent work has included the introduction of GDP synthesis models (90, 192, 193), rigorous models and solution methods (45, 91, 194), and thermally integrated models (195, 196) for distillation columns (see Figure 12).

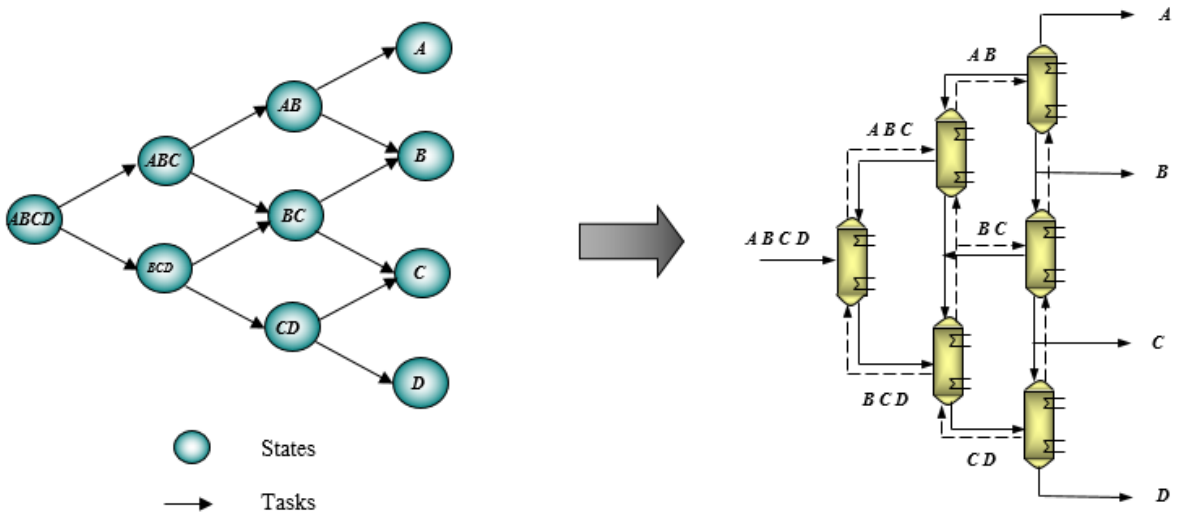


FIGURE 12: STN DISTILLATION SYNTHESIS SUPERSTRUCTURE FROM (195)

Within distillation network synthesis, the design of reactive distillation configuration is a popular topic. Okasinski & Doherty explain how reactive distillation can bring economic benefits by decreasing required investment costs, exploiting synergies between the reaction and separation, and simplifying the flowsheet (197). Siirola provides a classic case study for the benefits of reactive distillation (198). Superstructures and models for reactive distillation have been developed by multiple authors (83, 199–201). As a result of its popularity, many good reviews are also available for reactive distillation (202–205).

Mass exchange and water networks

Research into synthesis of mass exchange networks (MENS) arose to address the design of waste treatment systems (18). In the limiting case of single-component concentration targets, the MENS problem has several similarities to the HENS problem, with analogous driving forces in concentration and temperature. As with HENS, an LP targeting model is available (206), as well as an MILP transshipment model and MINLP utility cost problem (207). Kovacs et al. introduced global optimization of MENS superstructures (208). As with HENS, heuristic methods based on pinch analysis also exist for MENS (209), with the most highly cited papers in water network synthesis (a subset of MENS) dominated by heuristic modeling and optimization methods. Recently, the topic of water network synthesis has gained additional prominence due to growing awareness of diminishing freshwater supplies and the need to reduce utilization rates (210). Wang & Smith and Kuo & Smith introduced a graphical approach to superstructure optimization of water networks (211, 212). Later, Alva-Argaez and coworkers introduced an iterative MILP solution strategy (213) for the model in (211), and Galan & Grossmann give an approximate global optimization strategy for the same (214). Recent work in water treatment networks has included new rigorous MINLP/GDP models and solution strategies for global optimization (215, 216) (see Figure 13). Recent trends for MENS have included a move towards incorporating both mass and heat integration in processes (217–220). A review of combined water and energy integration can be found in (221).

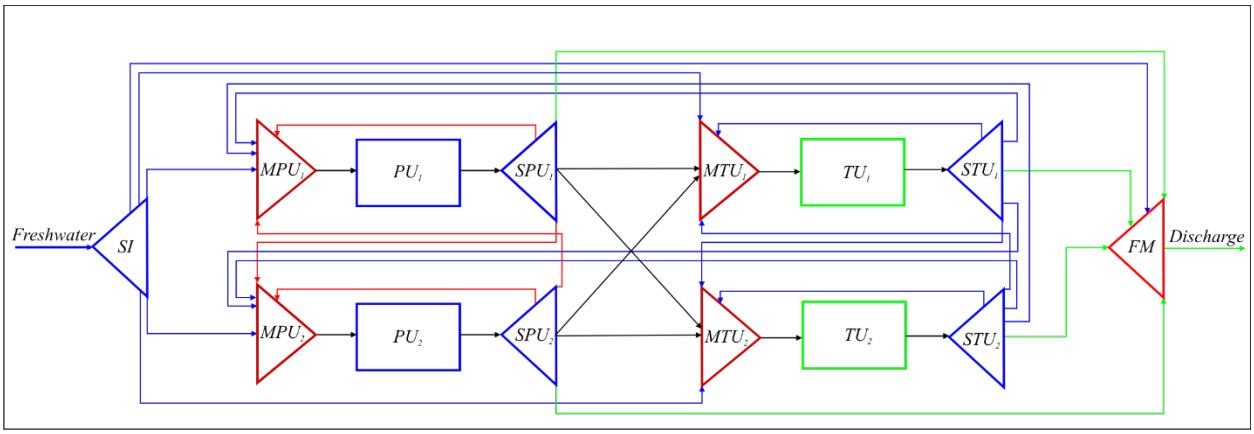


FIGURE 13: WATER NETWORK SUPERSTRUCTURE FROM (215)

Reactor networks

The mathematical programming approach to reactor network synthesis relies on the combination of two strategies: targeting and superstructure optimization. Key to the targeting problem is the concept of an "attainable region"—the convex hull of concentrations achievable from the feed through reaction and mixing operations (222). Glasser et al. and Hildebrandt et al. developed a geometrical method for obtaining the attainable region given a feed concentration (223, 224) (see Figure 14). Later, some characteristics of the attainable region were given in (225). Solution of the targeting problem yields an achievable bound on system performance that does not rely on a selected reactor configuration. This knowledge informs the generation of a superstructure that includes the optimal structure. Early targeting models were developed by various authors (79, 226). A state-space approach was presented by Burri et al. (227). Contributions for superstructure optimization include (228, 229). More recently, Esposito & Floudas present a global optimization approach to isothermal reactor network synthesis (230).

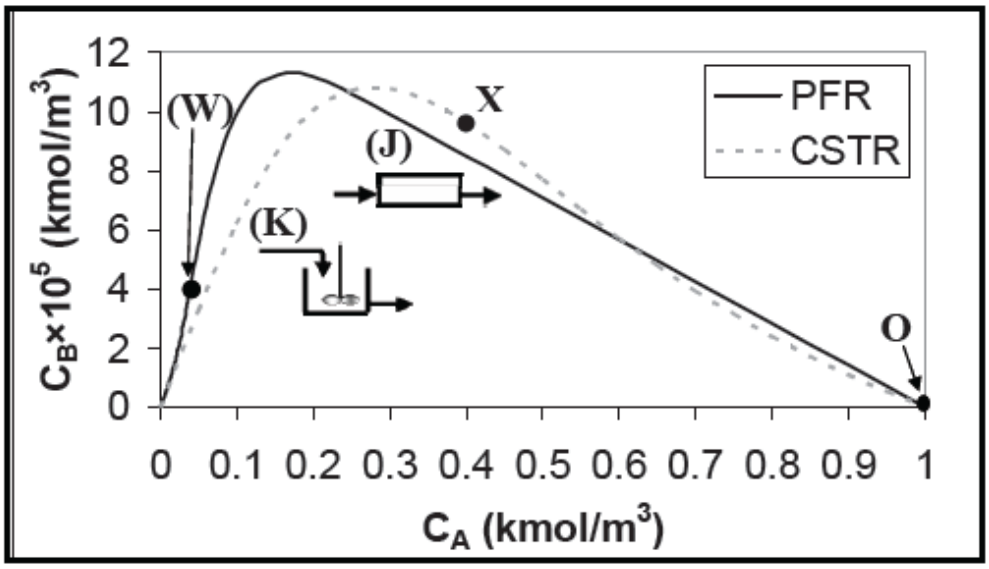


FIGURE 14: ATTAINABLE REGION EXAMPLE, FIGURE FROM (224)

Process Flowsheets

Most computational tools for process flowsheet synthesis continue to be based upon the hierarchical decomposition approach, rather than a mathematical programming one. With hierarchical decomposition (231), the synthesis process is divided into five decision levels: 1) batch vs continuous, 2) input-output structure, 3) recycle structure and reactors, 4) separation systems and 5) heat exchanger network. The method progresses through these decision levels sequentially. Heuristics, shortcut design procedures, and engineering intuition guide design choices made at each decision level that are then imposed upon subsequent decision levels. The result is a base case design that can be subsequently modified. Among the most prominent implementations of hierarchical decomposition are PROSYN (232) and ICAS (233). PROSYN relies on a set of heuristic rules and expert systems for flowsheet elements to walk the end user through the design process. In contrast, ICAS is built upon an equation-oriented process simulation framework with various toolboxes aimed at addressing specific design problems, such as sustainability analysis (234).

In contrast to the hierarchical decomposition approach, mathematical programming simultaneously optimizes at multiple decision levels, providing both the configuration and operating levels of the optimal process. This can lead to synergies not obvious in a sequential design approach (167, 168). With mathematical programming, binary variables (0-1/true-false) denote presence or absence of units in the superstructure of process alternatives. Modeling and solution approaches to flowsheet synthesis have focused on exploiting the special structure of synthesis problems: specifying the process configuration typically leaves only continuous variables, yielding an NLP. The DICOPT outer-approximation algorithm and its refinements (93, 143, 235, 236) iteratively optimize the continuous variables for a fixed configuration and select the next configuration using an MILP master problem with linearizations based upon the previous NLP sub-problem solutions. However, this algorithm is susceptible to becoming trapped in local solutions for nonconvex problems due to singularities introduced by zero value flow rates through non-selected process unit models. The Modeling/Decomposition strategy introduced by Kocis & Grossmann (84) attempts to address this issue by solving the NLP sub-problem only for selected units and interconnections in the superstructure. One of the only existing software packages developed for mathematical programming based flowsheet synthesis, MIPSYN (originally named PROSYN) (237–239), uses this strategy.

In order to leverage existing flowsheet simulators, various authors have also attempted to integrate mathematical programming techniques with simulation software (239–241). A recent contribution involves the use of Kriging surrogate models for various process units (242).

With a mathematical programming approach, the introduction of logic-based methods and Generalized Disjunctive Programming (GDP) enables much more structured model formulation and solution strategies. A summary of the advances in GDP are given in previous sections, but the most promising developments are Logic-based Outer-Approximation (85) and its global optimization counterpart (103). These strategies formalize the reduced space NLP technique introduced in (84) and thus effectively sidestep zero-flow-related difficulties in model solution. Recent work on cutting planes (104), redundant constraints (243), and logical reformulations (96) have also improved the tractability of global optimization for a variety of process networks.

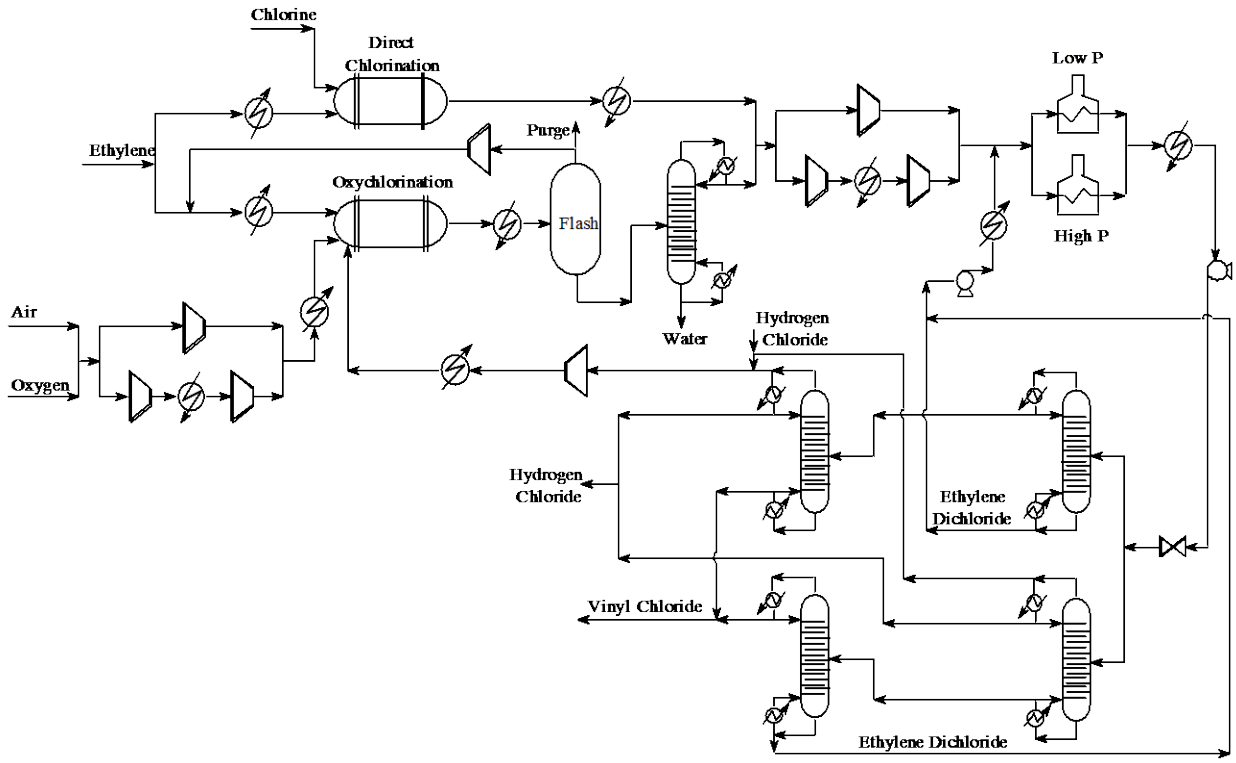


FIGURE 15: PROCESS FLOWSHEET SUPERSTRUCTURE, FIGURE FROM (86)

Critical Assessment

Although there has been significant progress in optimization-based process design, several challenges in implementation and theory deserve more attention. In many areas, theory has made great advancements, but the progress is not reflected in commercial packages; that is, academic impact has not translated into industrial impact. Harmsen gives a blunt opinion on penetration of mathematical programming-based synthesis tools in industrial practice: “So far the industrial [community] does not apply the method for generating completely new process designs” (244). One reason for this gap is that there is a lack of a general-purpose mathematical programming synthesis tool akin to Aspen for flowsheet simulation.

Few computational tools are available to tackle the general conceptual design problem. ICAS is a thermodynamics- and decomposition-driven toolset allowing for generation of alternatives, but it does not guarantee rigorous optimality (245). Similarly, PROSYN relies on heuristics and expert systems (232). MIPSYN performs superstructure optimization using a mathematical programming-based approach (246), but its codebase has become dated. PNS Editor, though able to handle multi-period problems, is restricted to linear constraints with fixed costs (247), precluding use of rigorous models. Many other attempts at toolmaking over the years are no longer in active development or have not gained enough attention (11, 248, 249). There are multiple options available to close this gap. One way is to incorporate more mathematical programming techniques into existing industrial tools. The LP and MILP solver community has been particularly successful in this regard, with Gurobi recently announcing a partnership with the SAP business intelligence toolset (250). Academic efforts have also been made to integrate MINLP solution tools with flowsheet simulators, including early work by Lang & Biegler (251) as

well as a recent contribution by Caballero et al. (92). Another strategy is the creation of a general-purpose synthesis tool for widespread adoption. This approach involves many challenges of its own, including the need to be user-friendly and approachable for novice modelers. In this endeavor, the shift towards Object Oriented Modeling and Generalized Disjunctive Programming will be a key asset, providing the ability to easily define and connect common flowsheet building blocks and abstract away the variable, constraint, and disjunction definitions behind a higher level programming object or a diagram of a distillation column on the screen.

Continued theoretical development of optimization-based process design methods is also important, including in the area of global optimization (41). Global optimization provides decision-makers with a mathematically rigorous assessment of the solution quality by providing a bound on the performance of a feasible solution to the given mathematical model. Unfortunately, current general purpose techniques are limited in terms of the problem sizes for which bound convergence is possible in a practical timeframe. Specialized algorithms designed to exploit particular problem structures expand the range of tractability, but these algorithms frequently need to be fine-tuned to the specific application and they may still be limited by the need to develop model approximations.

Theoretical advances are also needed to address the challenge of rigorous models, or more broadly, the incorporation of multi-scale information in the design process. Physical or chemical phenomena at the micro-scale may influence the performance of a unit model at the design level in nontrivial ways. Accounting for these effects may require addition of many variables and constraints to the superstructure model or the development of reduced-order models (252). Both of these approaches would benefit from increased attention. Surrogate models have garnered the most recent attention as a way to address this need (242, 253). Systematic methods for deriving surrogate models such as ALAMO (254) show great potential for allowing consideration of detailed phenomena at the process synthesis level.

Although process intensification holds much promise, design of intensified processes remains a theoretical challenge. In particular, work is needed to determine how to postulate superstructures for intensified processes such that a minimal coverage of the feasible alternatives is obtained. Different authors have proposed the use of phenomena-based building blocks as the fundamental components for designing a process (34, 255). Superstructures based upon these phenomena-based blocks are able to represent intensified processes, but few methods are available to determine which and how many phenomena blocks are needed to represent available alternatives. Furthermore, it is not yet established how to determine the optimal configuration of phenomena blocks because assignment of phenomena into tasks or equipment is needed in order to determine the value or cost of groups of blocks. One possible approach is to treat the system as a bilevel program, where the upper level decisions involve selection and configuration of the phenomena blocks while a lower-level optimization program groups the blocks into tasks or equipment and provides pricing information. However, this class of problems is very difficult to solve, with algorithms for the general nonconvex bilevel MINLP only recently becoming available (256, 257) and restricted to smaller problem sizes. Recent heuristic methods for synthesis sidestep this challenge, but opportunities exist for rigorous mathematical programming approaches to the problem.

Another challenge associated with synthesis of intensified processes is the need to use rigorous models to properly characterize the detailed chemical and physical phenomena exploited for intensification. For

example, in reactive distillation, the rate of reaction may depend strongly upon the temperature at each stage rather than any aggregate measure. An accurate depiction of process characteristics would also be necessary to determine viability of intensification based upon task integration.

Retrofit design also remains a substantial challenge for process synthesis. A review by Grossmann et al. from 1987 (258) lays out many unique difficulties of retrofit design that are still relevant today. Compared to green-field design, the retrofit problem can be much more challenging, with a larger search area in design space and inclusion of high-fidelity models for existing equipment. Whereas in green-field design, equipment can be represented by a model for its nominal performance, retrofit design may need to consider intricacies related to the internal geometries of current process units or other such details. Existing plant layout and piping may lead to other limitations that are not typically considered in green-field design, such as space availability on piping racks. Work on retrofit design has focused primarily on heat exchanger networks, with initial work in (259–261) and more recent contributions in (262, 263); there are also some recent contributions in water networks (210, 264). Opportunity exists to generalize current methods for other subsystems and for general process flowsheets.

Theoretical challenges are also present for methods to handle uncertainty in process parameters or requirements. Traditional approaches have centered upon feasibility and flexibility analysis of processes (48, 49, 265). Another possible approach is two stage stochastic programming, which could exploit the natural time gap between design and configuration of a process in the first stage and the start of operations in the second stage (50). Multi-stage stochastic programming incorporating future expansion opportunities would be a natural extension. However, these approaches would increase the complexity of an already difficult design problem. Therefore, new theoretical advances are needed to ensure that these techniques are tractable for relevant-sized problems.

Future Challenges

Sustainability-oriented initiatives, in addition to the more traditional profit motive, are likely to drive demand for process design research in the future. One such initiative is the incorporation of biomass as a chemical and energy feedstock. While corn-based ethanol featured prominently in the first generation of bio-based feed stocks, there is growing interest in fuel production from algal or non-food crop sources. Furthermore, conversion of biomass to chemical precursors for plastics production or other uses is also an active area of study. As these technologies gain maturity, scale-up and process design will become active considerations. Due to the transportation costs of biomass, research is also needed to determine whether a distributed versus more traditional centralized manufacturing system is best (266). Design of alternative energy systems will also be a growth area. Process alternatives for carbon capture power generation facilities need to be evaluated and optimized so that existing sources of energy can be consumed while mitigating the impact on the environment. Integration of new renewable power sources such as wind and solar into existing energy networks also continues to be a challenge (267), with research needed to ensure grid reliability and mitigate the unintended consequences of generation volatility.

At the same time, increased production of shale gas in the US and other regions introduces new demand for C1 and C2 chemistry flowsheets. With low-cost and plentiful shale gas available both as a feedstock and as an energy source, chemical producers are looking to expand their existing operations and

construct new facilities. These developments provide new opportunities to put recent conceptual design theory into practice.

Another area of rising consequence is modular and distributed manufacturing. These complementary concepts introduce a new angle to economies of scale. Taking advantage of process intensification (268), the aim is realize economies of scale not by building a world-scale continuous or batch facility, but by mass-production of small-scale modular continuous plants (269). These modular plants benefit from the efficiency of a continuous process while retaining flexibility characteristic of a batch process, due to the ability to reconfigure inter-compatible process modules (270). Modularity also allows for these plants to be quickly designed and constructed, decreasing payback periods and speeding up time-to-market for new products (271). By distributing these plants to sites near either customers or key feedstocks, significant logistical cost reductions are also possible. Locating a plant next to a customer also allows for increased responsiveness to evolving customer needs. Altogether, this new style of manufacturing shows great promise for delivering the short design lead times to address market variability and the production efficiencies to address intensified global competition (271).

Finally, recent advancements in spaceflight promise to spark a new era of extra-terrestrial commercial activity, with new opportunities for process design. Already, significant investments in extra-planetary industrial activity are being made in the area of asteroid mining (272). While in the near term this activity will be restricted to precious compounds brought back to Earth for processing, interest will grow for the ability to perform some processing activities in space and avoid the significant transportation costs. Efforts to place human settlements on the moon and Mars will also require local processing of resources, both to sustain habitable conditions and to provide materials for expansion and development. The designs for these emerging applications will face different challenges than earthbound processes, both in the key objectives as well as in the necessary constraints. For example, processes destined for launch will face stringent mass and volume limitations given current rocket technology. However, developments on the ground can also have an effect. For example, advances in PI may be a powerful tool for expanding viability of extra-terrestrial processing. Regardless of where they are applied, many of the principles of design (273) will hold true, wherever the final process—on the ground, in orbit, or out of this world—and so they will remain key lessons for future generations of engineers.

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