Review of mixed-integer nonlinear and generalized disjunctive programming applications in Process Systems Engineering

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1 Introduction

In this chapter we present some of the applications of MINLP and generalized disjunctive programming (GDP) in process systems engineering (PSE). For a comprehensive review of mixed-integer nonlinear optimization we refer the reader to the work by Belotti et al.[1]. Bonami et al.[2] review convex MINLP algorithms and software in more detail. Tawarmalani and Sahinidis[3] describe global optimization theory, algorithms and applications. Grossmann[4] provides a review of nonlinear mixed-integer and disjunctive programming techniques. A systematic method for deriving MINLP models through GDP is provided by Grossmann and Trespalacios[5]. For a detailed review of MINLP solvers we refer the reader to the work by Bussieck and Vigerske[6] and D'Ambrosio and Lodi[7].

One of the main concepts in optimization in PSE is the idea of superstructure. A superstructure contains most (or all) of the alternatives a system can have. Superstructures are defined by the modeller, and alternative superstructures can be derived for the same process. The mathematical optimization approach seeks to find the optimal configuration of the proposed alternatives. For a more comprehensive description on superstructures, we refer the reader to the work by Grossmann et al.[8]. The online library of problems www.minlp.org contains several PSE problems and includes a detailed description of the model, application, and the MINLP problem formulation.

Different type of models have been used for different PSE applications. Table 1, adapted from Biegler and Grossmann[9], provides an overview of the different types of models used in the different PSE applications. The different models in Table 1 are: linear programs (LP), mixed-integer linear programs (MILP), linear generalized disjunctive programming (LGDP), quadratic programs (QP), linear complimentary problems (LCP), nonlinear programs (NLP), mixed-integer nonlinear programs (MINLP), and generalized disjunctive programming (GDP). This chapter presents a review on the applications that require the use of MINLP and nonlinear GDP models.

Table 1: Applications of mathematical programming in process systems engineering

	LP	MILP/LGDP	QP, LCP	NLP	MINLP/GDP
Process synthesis					
Process Flowsheet		✓		✓	✓
Reactor Networks	✓			✓	✓
Separations		✓			✓
Heat Exchange Networks	✓	✓		✓	✓
Water Networks	✓	✓		✓	✓
Operations					
Planning	✓	✓			✓
Scheduling	✓	✓			✓
Real-time optimization	✓		✓	✓	
Process control					
Linear MPC	✓		✓		
Nonlinear MPC				✓	
Hybrid		✓		✓	✓
Molecular computing		✓			✓

2 Process synthesis

In this section, we present a summary some of the main applications of MINLP and GDP in process synthesis. Grossmann et al.[8] provide a comprehensive review on the development of optimization models and methods in process synthesis.

Process Flowsheet Synthesis. MINLP has been widely used for process flowsheet synthesis. The problem seeks to obtain the optimal configuration of a process contained in a given superstructure[10–12]. The superstructure contains alternative units, interconnections, and process properties. The selection of units and their interconnections are modeled using binary variables, while the properties of the process (flow, concentration, etc.) are modeled with continuous variables. Alternative superstructure representations of processes have also been proposed[13–16].

Process flowsheet synthesis is one of the areas where GDP has been most successful. Raman and Grossmann[17] proposed a GDP model for process flowsheet synthesis. Disjunctive programming techniques for the optimization of process systems with discontinuous investment costs-multiple size regions were presented by Turkay and Grossmann[18]. These authors[19] also presented logic-based MINLP algorithms for the optimal synthesis of process networks. Later, Yeomans and Grossmann[20] formulated with GDP the two fundamental superstructures for process systems (state task network and state equipment network). GDP methods have shown to improve solution times for linear, convex and nonconvex process flowsheet synthesis problems[20–24].

The accurate modeling of a process flowsheet, including the detailed formulations of each unit, normally

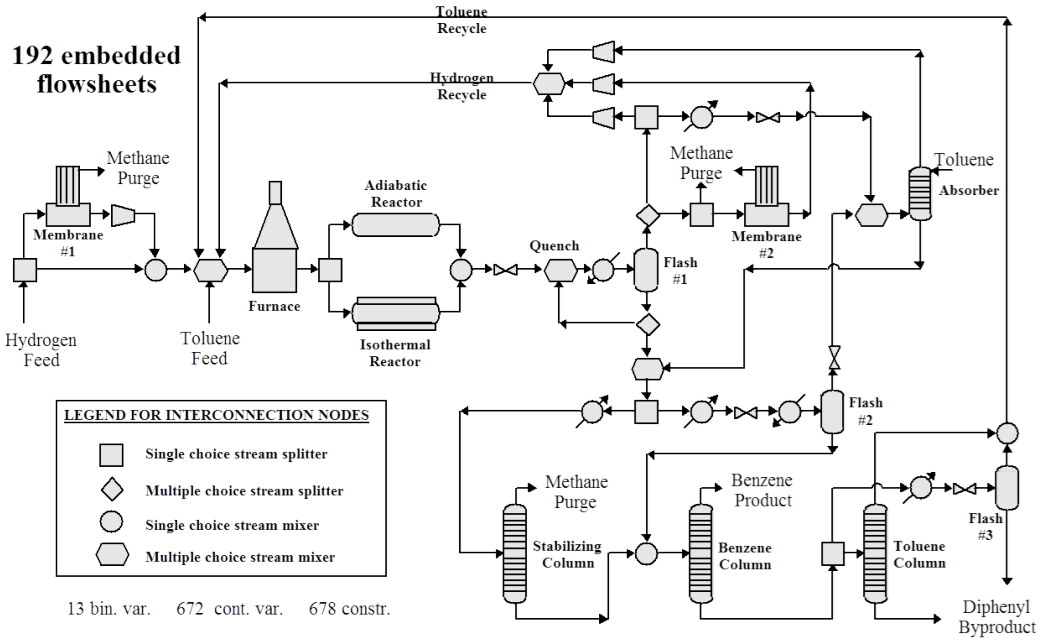

Figure 1: Process flowsheet superstructure for the HDA process

yields a large scale nonconvex MINLP. There are two general frameworks that are normally used to tackle these problems: decomposition techniques[25–28], and surrogate models[29–32]. There are many processes in which flowsheet optimization has been applied over the last 30 years. The most recent work has focused mainly on bioenergy systems and biorefineries[33–42], polygeneration systems[43–45], and gas-to-liquid complexes[46].

Figure 1 presents a process flowsheet superstructure for the hydrodealkylation of toluene (HDA) process[25]. The given superstructure contains 192 different flowsheets. The figure shows the possibility of selecting alternative connections and units, such as adiabatic or isothermal reactors, membranes, absorber, distillation columns, flash units, compressors, heat exchangers and valves.

Reactor Network. This problem seeks to optimize the configuration of a reactor system for a given feed and a given set of reactions. There are two main mathematical programming approaches for this problem: superstructure optimization and targeting. A review of both methods is provided by Hildebrandt and Biegler[47].

Superstructure optimization methods require the modeler to postulate a superstructure, which represents possible configurations for the reactor network. This structure is formulated as an MINLP and solved with optimization tools. Achenie and Biegler[48] postulated a superstructure NLP model. The continuous model allows the selection of the network structure, reactor type, and amount of heat addition. This model uses a dispersion coefficient to determine the reactor type. Later, the same authors postulated an alternative NLP which uses the recycle ratio as the determinant of reactor type[49]. Kokossis and Floudas[50–52] presented

a superstructure of CSTRs and PFRs. In the MINLP, the PFRs are modeled as a series of CSTRs, which eliminates the use of differential equations in the model. Smith and Pantelides[15] presented a reaction and separation network with detailed unit operation models. Esposito and Floudas[53] make use of the global optimization tools to solve a nonconvex MINLP in which the PFRs of the superstructure are modeled using differential algebraic equations.

The targeting method seeks to identify the maximum possible performance. A reactor network that meets this criteria is then determined. Horn[54] introduced the concept of "attainable region". Attainable region is the convex hull of possible concentrations for a given feed and reaction scheme. The geometrical concepts that allow the derivation of the attainable region, and further extensions to higher dimensions where developed mainly by Glasser, Hildebrandt, and Feinberg[55–58]. Burri et al.[59] applied the Infinite DimEnsionAl State-space (IDEAS) framework to construct the attainable region of reactors. This framework was also used by Zhou and Manousiouthakis[60] and Davis et al.[61] to find the attainable region of non-ideal reactors and of non-steady-state networks of batch reactors. There are two main downsides of the "attainable region" technique. The first one is that since it is a graphic method, it can handle at most three dimensions. The second one is that every time that the conditions for the reactor problem change, the region must be recalculated. To solve this issues, and improve the performance of the method, Biegler et al.[62–66] developed hybrid methods that combine "attainable region" with optimization techniques.

Single Distillation columns. The simplest distillation design problem is to select the feed tray location in a distillation column with a given number of trays. The superstructure of this problem was postulated by Sargent and Gaminibandara[67] for ideal mixtures, and extended later for azeotropic cases[68] (see Figure 2a). Viswanathan and Grossmann[69] presented the superstructure of a distillation column in order to optimize not only the feed tray, but also the number of trays in the column. (see Figure 2b) The model also allows the possibility of multiple feeds. This model was later incorporated into more comprehensive superstructures which incorporated thermodynamic components[15, 70], and thermally coupled distillation columns and dividing wall columns[71].

One of the main issues of the tray by tray MINLP model of a column is the large number of nonconvex constraints in the model. Yeomans and Grossmann[72] proposed a GDP model for the tray by tray representation of the column, as well as for the sequence superstructure. They proposed a logic-based Outer Approximation approach, which considerably reduces the number of nonconvex constraints in each iteration. Based on the tray by tray GDP model, Barttfeld et al.[73] presented a computational comparison between the MINLP and GDP models using a heuristic algorithm, showing the advantages in solution times of the GDP model.

Distillation sequences. The separation problem was originally defined more than 40 years ago by Rudd and Watson[74]. For the MINLP and GDP applications, Yeomans and Grosmann[20] characterized two major

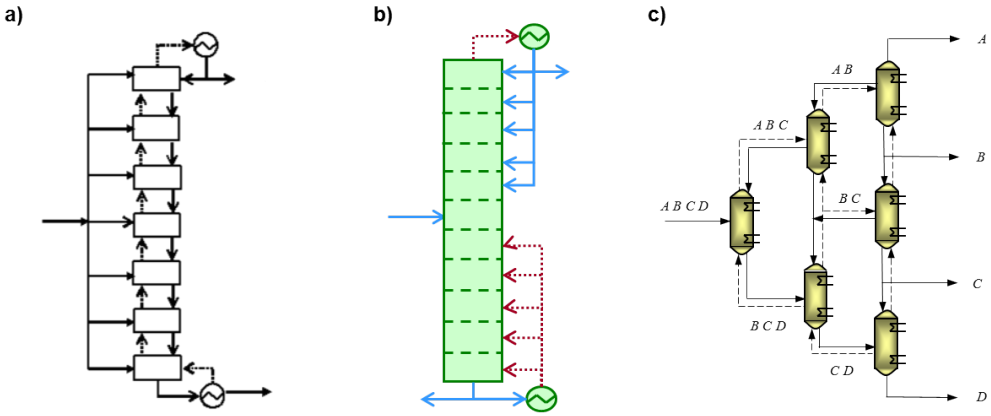

Figure 2: Superstructures for a) Feed tray location. b) Feed tray location and number of plates. c) distillation sequence for a 4 component zeotropic mixture.

types of superstructure representation: State-Task-Network (STN) (see also Sargent and Gaminibandara[68]) and State Equipment Network (SEN) (see also Smith and Pantelides[75]). They described both representations using GDP models.

For sharp split columns, the superstructure can be modeled as an MINLP. The GDP formulation for the STN model is straightforward[76]. In the case where each column is assigned to each of the split separation tasks, the model reduces to the MILP superstructure proposed by Andrecovich and Westerberg[77]. The SEN structure is not as straightforward, but it is numerically more robust[72, 76]. Novak et al[78] used this representation before being formalized by Yeomans and Grosmann[20].

In order to develop more efficient distillation sequences, heat integration between different separation tasks can be considered. Paules and Floudas[79, 80] proposed an MINLP model for heat integrated distillation sequences, and Raman and Grossmann[17] a disjunctive representation.

Thermally coupled systems seek to reduce the inherited inefficiencies due to the irreversibility during the mixing of streams at the feed, top, and bottom of the column. The design and control of these columns are complicated, but they were made possible by the design concept of "thermodynamically equivalent configuration"[81–84], and the improvement in control strategies[85–89]. For zeotropic mixtures, Agrawal[90] characterized a subset of the possible configurations named basic configurations. This concept helps to reduce the search space of feasible configurations, since non-basic configurations normally have higher overall costs[91–93]. Algorithms for finding the basic configurations[103], and mathematical representations of these configurations have been proposed[94, 95]. In terms of GDP, logic rules that include all the basic column configurations have been developed by Caballero and Grossmann[91, 96, 97].

Figure 2c presents the distillation sequence superstructure for a 4 component zeotropic mixture, presented by Sargent and Gaminibandara[68].

Heat exchange networks. A comprehensive heat exchange network (HEN) review with annotated bib-

liography is provided by Furman and Sahinidis[98]. A more recent review on the developments of HEN is provided by Morar and Agachi[99]. Following the classification proposed by Furman and Sahinidis[98], the work in HENs is divided in sequential or simultaneous synthesis methods.

The sequential synthesis method decomposes the design of HEN typically in three simpler sequential problems, but it does not guarantee the global optimum of the HEN. The first problem seeks to minimize the utility costs. The second one seeks to minimize the number of heat exchange units, while satisfying the minimum utility cost previously found. The last problem minimizes the network cost subject to the minimum number of units found. The first problem (minimizing utility usage/cost) can be an LP[100–102], an MILP[103, 104] or an MINLP[105]. The second problem is an MILP[100, 101, 106, 107]. The most common model for the third problem that minimizes the network cost is an NLP[108].

In simultaneous synthesis the HEN is optimized without decomposing the problem. One of the first MINLP models was presented by Yuan et al.[109], describing a superstructure of the network. This MINLP, however, does not allow the splitting or mixing of streams. The work by Floudas and Ciric[110–113] presents an MINLP model that optimizes all of the costs of a HEN without the need of decomposition. Yee and Grossmann[114, 115] presented a linearly constrained MINLP formulation of a multi-stage superstructure that allows any pair of hot and cold streams to exchange heat in every stage. The superstructure of this model for two possible stages is shown in Figure 3. This model was extended to include flexibility[116–118], detailed exchanger design models[119, 120], and isothermal streams involving phase change[121].

The simultaneous optimization of process flowsheet and heat integration was addressed by Duran and Grossmann[122] through a set of nonlinear inequalities. Particular applications of heat integration with optimization of distillation columns and distillation sequences where addressed earlier in this section. Grossmann et al.[123] presented a GDP model for simultaneous flowsheet optimization and heat integration. Recently, Navarro-Amoros et al.[124] extended this GDP model for heat integration with variable temperatures.

Utility systems. Petroulas and Reklaitis[125] proposed a mathematical optimization model for the design of utility systems, based on an LP and a dynamic programming approach. An MILP model was formulated by Papoulias and Grossmann[126], which assumed linear capital costs with fixed charge and linear energy balance. Bruno et al.[127] proposed a refined version of this model by including nonlinear functions, presenting the first MINLP model for the design of utility systems. The superstructure of this MINLP is shown in Figure 4. This MINLP involves nonlinearities to represent the cost of equipment and the plant performance in terms of enthalpies, entropies and efficiencies. The model considers steam properties at specific pressures, so it cannot simultaneously optimize the operating conditions of the steam levels. Savola et al.[128] presented a modified MINLP model that allows the simultaneous optimization of pressure levels, by using correlations that depend on both pressure and temperature.

Water Network. A comprehensive review of water network design methods with literature annotations

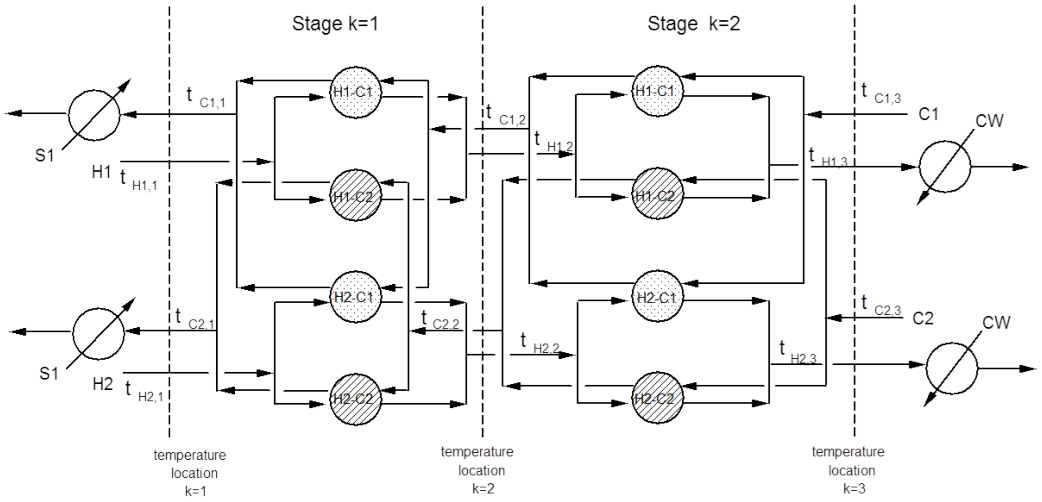

Figure 3: Superstructure of multiple stages with potential heat exchangers

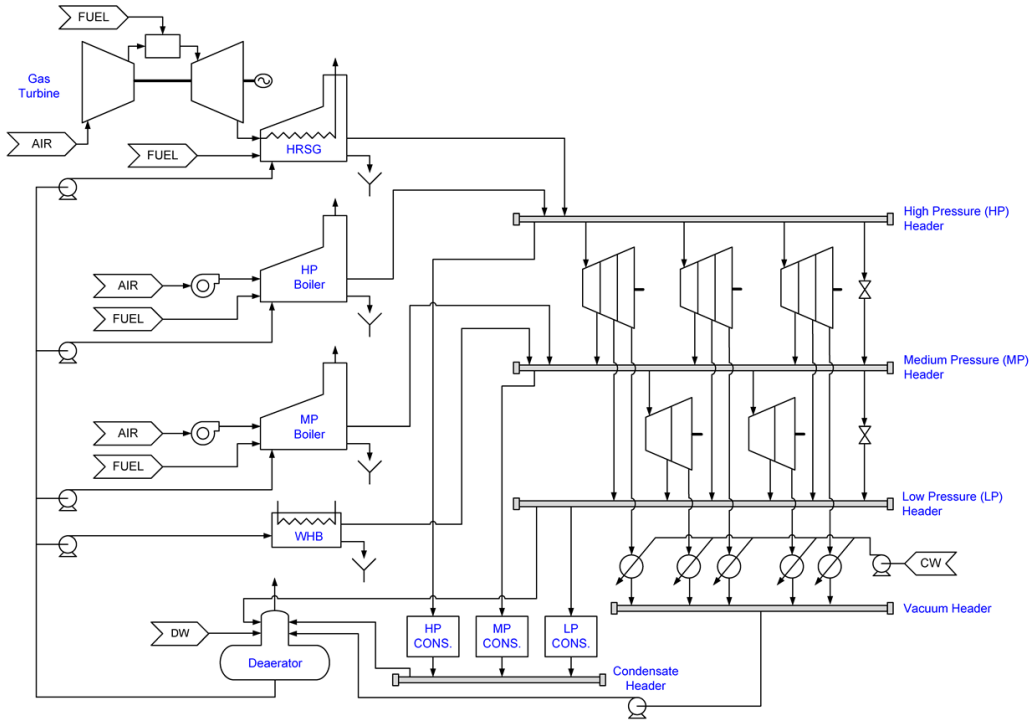

Figure 4: Superstructure for utility plants

is provided by Jezowski[129]. The optimization based methods for water network design are based on superstructures, which encompasses most (or all) feasible solutions for the network. There are four types of water networks that are normally modeled. The network of water-using processes is called water-using network (WUN). The second type is the wastewater treatment network (WWTN). These two networks are subsystems of the third type of network: the total water network (TWN)[130, 131]. Finally, the fourth type is the complete water network (CWN), which is a TWN with pretreatment units[132]. The models in water networks typically seek to optimize the configuration of the network and units operating conditions, satisfying the water quantity and quality requirements in the WUN, with water discharges within the environmental restrictions.

The superstructure based optimization of the WUN is relatively simple, due to the fixed number of water using units. However, the use of alternative water treatment units in WWTN, TWN, and CWN makes the problem more complex. In particular, the mixing of streams yields bilinear terms (which are nonconvex), and the operating constraints in each of the units may be highly nonconvex. In addition, the selection of units and interconnections are represented by binary variables. The combination of these constraints and variables result in a nonconvex MINLP. The WWTN alone has been shown to be a very difficult problem, equivalent to the generalized pooling problem[133].

The first MINLP model for the simultaneous global optimization of water networks was presented by Karuppiah and Grossmann[134], which is derived from a GDP formulation. This model was extended by Ahmetovic and Grossmann[135] to include all feasible connections between one or multiple sources of water of different quality, water-using processes, and wastewater treatment operations. Since the MINLP that arises in water networks is difficult to solve, five strategies are normally used for solving the problem. The first one is the linearization of constraints, typically used for the WUN. The first linearization was developed for a single-contaminant problem[136], and its optimality constraints were derived by Savelski and Bagajewicz[137]. The model was later extended for multiple contaminants[138], though the conditions are different[139], and it requires a specialized branching approach. Other linearization techniques for WUN with regeneration processes[140], near-optimal single stage method for WUN with multi-contaminant[141], and WWTN[142] have been presented. The second approach is to find good solutions (locally optimal) through good initial points. A common practice is to fix the outlet concentrations at the maximum values[143, 144]. The third approach is to use sequential optimization, originally presented by Takama[145]. Some of the sequential optimization approach methods include: a relaxed NLP model[146], dividing and sequentially reducing concentration intervals for WUN[147], an MILP-LP technique for TWN[148], and an LP-NLP approach for the WWTN[149]. The fourth strategy is to solve the MINLP problem by using meta-heuristic algorithms[150–152]. The last approach is to solve the MINLP problem using rigorous global optimization techniques[134, 135, 153].

Dong et al.[154–158] have recently proposed MINLP models that incorporate the design of heat exchange

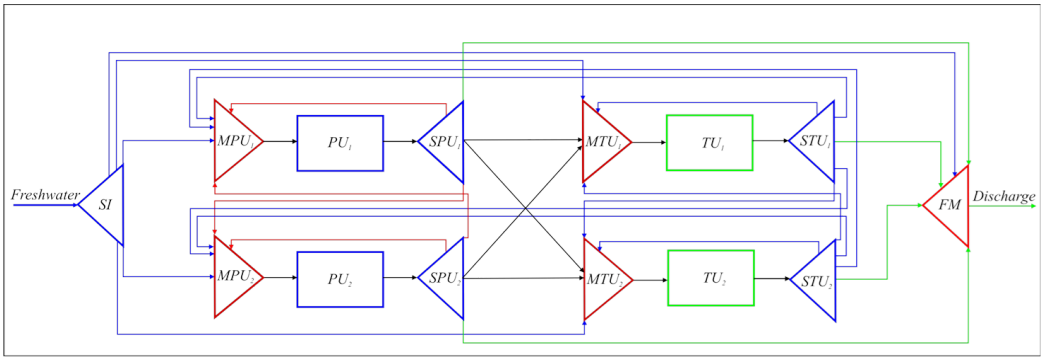

Figure 5: Superstructure of integrated water network with two process and two treatment units

networks with water networks, based on the state-space superstructure proposed by Bagajewicz et al.[159, 160]. Ruiz and Grossmann[161] present a simplified GDP formulation of the WWTN, as an illustration of the bound tightening technique.

Figure 5 presents the superstructure of a water network[135] with one source, one discharge, two water using processes and two treatment units. It can be seen from the figure that all possible connections between the water using units and water treatment units are considered, including recycle streams.

3 Planning and Scheduling

Process planning and scheduling has been an area of much interest for industry and research over the past decades[162–165]. Although the boundary between planning and scheduling is sometimes not clear, time scale provides a distinction between the two. Planning normally involves medium-term (e.g. year, quarters, months or weeks) decisions such as assignment of production tasks to facilities and transportation logistics. Scheduling defines short-term decisions such as assignment of tasks to units, sequencing of tasks in each unit, and determining starting and ending times for the execution of tasks. A review of planning and scheduling in the process industry is provided by Kallrath[163]. Models and techniques to integrate planning and scheduling have also received attention in recent years[166]. In this section we present some of the main MINLP applications for planning and for scheduling.

Planning. Planning models are usually not as detailed as scheduling models, so most planing models are represented using MILP formulations[162]. However, refinery planning is one of the few areas where nonlinear models have been used. Moro et al.[167] presented an NLP planning model for diesel production refineries, extending it later to petroleum refineries[168]. Zhang at al.[169] presented one of the first MINLP models for refinery planing, which simultaneously optimizes liquid flows and allocation of utilities (hydrogen, and steam and power flows). They deal with the nonlinear terms by using picewise linear approximations. Elkamel et al.[170] presented an MINLP multiobjective model for the refinery planning, seeking to

maximize profit while reducing CO_2 emissions. Neiro and Pinto[171] presented an MINLP implementation for multiperiod refinery planning models using empirical relations. Alattas et al.[172] presented a multiperiod MINLP model that utilizes a more precise representation of the crude distillation unit, using the model introduced by Geddes[173]. Shah et al.[95] provide a literature review on approaches that address the problem of enterprise-wide optimization in the petroleum industry.

Scheduling. Many scheduling models assume process simplifications, and can be modeled as MILP[165, 174–176]. Castro and Grossmann[177] presented the traditional MILP formulations as a derivation of GDP models. Many applications, however, require the use on nonlinear constraints to better represent the process.

There are two non-process related cases that typically introduce nonlinearities to the traditional MILP representations. The simplest one is when cyclic schedules with infinite horizon are considered[178–182]. In this case, the objective function is divided by the length of the cycle time, yielding a linear fractional objective function. The rest of the model is represented using a traditional MILP representation. Specialized algorithms have been developed to address this problem[183, 184]. The second case is when a cyclic scheduling model includes average inventory equations[179]. The additional constraints in this case are nonconvex, and may require the use of a global optimization method for its solution[180, 181, 185].

In terms of process-related nonlinearities, blending equations are probably the most common type that appear in scheduling models[186]. These constraints make use of bilinear terms which are nonconvex in general, and lead to multiple local solutions. In order to solve this type of scheduling models to global optimality, rigorous global optimization techniques are used [187, 188].

One of the most complex nonconvexites in scheduling, arises in the modeling of dynamic processes. The dynamic, discrete and continuous behaviour of these systems give rise to mixed integer dynamic optimization (MIDO). This type of problems typically occur in the scheduling and control of polymerization reactors[189–193]. The the most common approach for solving MIDO problems is to discretize the system of differential equations through orthogonal collocation, yielding large scale MINLP models. Biegler[194] provides an overview of solution strategies for dynamic optimization.

4 Process control

Many processes in chemical engineering require the modeling of nonlinear systems, especially when representing dynamic behaviour. Additionally, discontinuity is expected in the operation and control of a process[195]. The dynamic models with mixed discrete and continuous variables are called hybrid systems (which are MIDO problems in general). Start-up and shut-down operations[196], batch systems[197], and grade transitions [192, 193] are some of the main applications of optimization of hybrid systems. Several hybrid formulations have been developed and implemented in recent years [198–205]. A comprehensive review

on modeling, simulation, sensitivity analysis and optimization of hybrid systems is provided by Barton and Lee[206]. Morari and Baric[207] present a review paper on developments in the control of hybrid systems.

GDP has also been relevant in the development of models and solution methods in hybrid systems. Oldenburg and Marquardt[204] developed a GDP model of "fixed alternative sequences", formalizing modeling approaches proposed by several authors[206, 208]. The authors solve the GDP model using a modified version of the logic-based Outer Approximation, showing the efficiency of the algorithm for finding global solutions. Ruiz-Femenia et al.[209] present a logic-based Outer Approximation algorithm for solving optimal control problems.

5 Molecular computing

A collection of works on computer aided design is provided by Achenie et al.[210]. The review paper on advances in global optimization by Floudas and Gounaris[211] provides several applications of global optimization in molecular computing.

From a mathematical programming perspective, one of the first works on molecular computing was developed by Macchietto et al.[212, 213]. The MINLP they proposed was based on group contribution accounting for the presence or absence of a group in a molecule. Churi and Achenie[214–216] further refined this model by incorporating some information on how the groups are connected to each other in the molecule. Naser and Fournier [217] proposed an alternative MINLP representation, and developed a heuristic method for solving the problem. All of these MINLP models and methods are solved using local tools, so they do not guarantee the global solution. Joback and Stephanopoulos[218, 219] proposed the use of interval arithmetic techniques, providing bounds on the properties of aggregate molecules, overcoming the multiple local optima issue.

Several applications of MINLP have been used in molecular design. Some of them include design of solvents[212, 214, 220–226], refrigerants[215, 216, 227–229], polymers[230–234], and pharmaceutical products[235, 236].

6 Concluding remarks

As can be seen from the review of this paper, mixed-integer nonlinear and generalized disjunctive programming techniques have had wide applicability in many problems in Process Systems Engineering. This has allowed not only a more systematic approach to the problems, but also one where optimal or near optimal solutions can be obtained. However, despite many successful applications, the global optimization of MINLP and GDP problems still remains a major challenge due to the limited problem size that can be handled with current methods.

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