Recent Advances in Computational Models for the Discrete and Continuous Optimization of Industrial Process Systems

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Abstract

An overview of the mathematical formulations used for discrete and continuous optimization are presented. These include Linear Programming, Nonlinear Programming, Integer Programming, Mixed-Integer Linear Programming, Mixed-Integer Nonlinear Programming, Logic-based Optimization, Stochastic Programming, Robust Optimization, and Flexibility Analysis. Successful applications of optimization models in industry are presented in the following fields: upstream oil & gas, materials blending, natural gas, biofuels, water treatment, electricity market integration, plant reliability, and supply chain design. Ongoing projects applying computational models to optimize industrial process systems are also mentioned. Implementations of customized optimization techniques that improve computational performance and enable finding solutions to otherwise unsolvable optimization problems are highlighted. These include strengthening cuts, decomposition strategies, model reformulation, and linearization, among others.

Keywords: Mathematical Programming, Enterprise-wide Optimization, Mixed Integer Programming, Generalized Disjunctive Programming, Stochastic Programming, Robust Optimization.

1. Introduction

Continuous and discrete optimization has played an important role in improving industrial processes. Since its origins, the field of optimization has been influenced by key researchers from the process industries. Among these are Martin Beale, Jacques F. Benders, Abraham Charnes, and William W. Cooper, who were key figures for applying mathematical programming in the oil industry. Beale joined the Corporation for Economic and Industrial Research (CEIR) in 1961, which later became Scicon (Scientific Control Systems Ltd.), where he led the development of mathematical programming software for industrial applications. (Beale 1965; Powell 1987). Benders joined the Shell laboratory in Amsterdam in 1955 and applied mathematical programming techniques to oil refinery logistics (Benders 1962). Charnes and Cooper were both affiliated with what is currently Carnegie Mellon University. Their research included applications of mathematical programming for aviation fuel blending in collaboration with Gulf Oil (Charnes et al. 1952; Cooper 2002).

The evolution of applied industrial optimization has led to the birth of a field called Enterprise-wide Optimization (EWO) (Grossmann 2005). EWO targets a more complete view of industrial processes that includes not only manufacturing, but also supply and distribution within the enterprise. There are different layers to EWO, namely, planning, scheduling, and control. These are depicted in the decision-making pyramid shown in **Figure 1**. The distinguishing element between the three decision levels is the time scale of the events involved. The control level pertains to the second to minute operational decisions at the manufacturing facilities, involving the manipulation of equipment and process parameters. The scheduling level involves decisions at the hours and days resolution such as the allocation of resources and event sequencing. The planning level is for long term decisions (weeks to years resolution) such as long-term investment decisions and operational targets. Within each level, optimization targets include profit maximization, improved resource utilization, cost minimization, and sustainable design and operation. Optimization in each of these decision levels can bring significant benefits to industries where implemented.

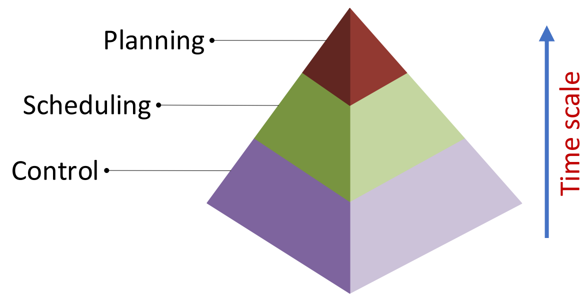

Figure 1. Decision-making pyramid for EWO

This paper is organized as follows, **Section** Error! Reference source not found. gives an overview of research focuses in the area of EWO at Carnegie Mellon University, highlighting industrial collaborations. **Section 3** presents an overview of the different types of continuous and discrete optimization models used for EWO. **Section 4** presents a total of 8 industrial applications areas for optimization. Concluding remarks are given in **Section 5**.

2. EWO Group

At Carnegie Mellon University, a multidisciplinary research center now known as the Center for Advanced Process Decision-making (CAPD) was established in the mid-80s by professors Art Westerberg, Larry Biegler, and Ignacio Grossmann. This center has grown since and is composed of researchers in the fields of chemical engineering, operations research, and industrial engineering. Its research goals include: 1) understanding and supporting complex issues faced by industry both from a design and an operational point of view, and 2) developing modeling and solution techniques to address those issues. Within the CAPD, there is an interest group that focusses on Enterprise-wide Optimization (EWO), whose goals include 1) optimizing entire supply chains, 2) developing novel planning and scheduling models that oftentimes address uncertainty, and 3) integrating planning, scheduling, and real-time optimization. A wide portfolio of projects has been undertaken over the years by the EWO group. Recent projects in the group along with the company collaborators are listed below.

1. Network design, planning, and scheduling
    a. Demand side management in the steel industry (*ABB*)
    b. New copper concentrate optimal scheduling topology (*Aurubis*)
    c. Unconventional oil gathering network design (*ExxonMobil*)
    d. Stochastic multi-period oilfield planning and design (*SKInnovation*)
    e. Integration of reservoir modeling with oilfield planning (*Total*)
2. Reaction systems
    a. Residue fluidized catalytic cracking real-time optimization (*Petrobras*)
    b. Continuous reactor design and optimization (*Dow*)
    c. Kinetic parameter estimation (*Eli-Lilly*)
3. Algorithms

    a. Stochastic nonconvex mixed-integer nonlinear programming algorithms (*ExxonMobil*)
    b. Design space via symbolic computation (*Eli-Lilly*)
4. Data driven approaches
    a. Polymer design with derivative-free optimization (*ExxonMobil*)
    b. Data-driven optimization of integrated chemical plants (*Dow*)
    c. Production schedule optimization with deep reinforcement learning (*Dow*)
5. Equipment and Maintenance
    a. Integrated reliability and storage design with maintenance policy optimization (*Linde*)
    b. Heat exchanger circuitry optimization (*MERL*)
    c. Advanced heat exchanger model optimization (*UTI Carrier*)
6. Supply Chain and Logistics
    a. Novel continuous-time inventory routing algorithms (*Air Liquide*)
    b. Multi-period vehicle routing algorithms (*Linde*)
    c. Full truckload delivery planning (*Braskem*)
    d. Customer service marginal cost estimation (*Air Liquide*)
    e. Digital supply chain business process optimization (*Dow*)
    f. Portfolio-wide optimization in the pharmaceutical industry (*Eli-Lilly*)

Industrial collaboration has been key to the research success and knowledge development in the EWO group. Industry driven projects have provided key insights that give real world relevance to the projects developed in the group. The knowledge gained from these collaborations is freely available to the public at http://egon.cheme.cmu.edu/ewo/seminars.html. In regard to the projects undertaken by the EWO group, most projects apply methods from mathematical programming, with increased emphasis on uncertainty. There has also been interest in other optimization approaches such as data-driven modeling, artificial intelligence, and symbolic computation.

The following section will provide an overview of the mathematical programming models used in discrete and continuous optimization.

3. Optimization Models

The general formulation for continuous and discrete optimization consists of an objective function and a set of constraints as shown in (**1**). The objective function f can be a linear or non-linear single-valued function. The optimization sense is usually minimization, although maximization can also be used. The set of constraints is given by linear or nonlinear sets of constraint inequalities and equalities. In the general notation given below, g_i is a vector-valued function of the variables x and y, which represent continuous and discrete variables, respectively. Other continuous and discrete sets besides m-dimensional reals and n-dimensional integers can be used for the domains of x and y. Binary variables are often used for the discrete variables to denote yes or no decisions.

$$\begin{aligned} \min_{x,y} \quad & f(x,y) \\ s.t. \quad & g_1(x,y) \leq 0 \\ & g_2(x,y) = 0 \\ & g_3(x,y) \geq 0 \\ & x \in \mathbb{R}^m \\ & y \in \mathbb{Z}^n \end{aligned} \tag{1}$$

Mathematical formulations can be divided into the following groups:

- Linear Programing (LP): all expressions are linear with respect to the variables, and only continuous variables are used. Algorithms for solving LPs fall into two categories: pivoting methods (e.g. simplex) and barrier methods (interior-point methods) (Tomlin 1989; Illés and Terlaky 2002).
- Nonlinear Programing (NLP): at least one nonlinear expression is used, and only continuous variables are used. Algorithms for solving NLPs fall into three main categories: 1) reduced gradient methods (e.g. GRG2, CONOPT, and MINOS codes), 2) successive quadratic programming (e.g. SQP code), and 3) interior point methods (e.g. IPOPT code) (Biegler 2010).
- Integer Programming (IP): all expressions are linear, and all variables are integer-valued. The two main algorithms for solving IPs are branch-and-bound (Dakin 1965), cutting planes (Balas et al. 1993), and branch-and-cut (Johnson et al. 2000). Many integer programs fall under the category of 0-1 IP, where all variables are binary.
- Mixed Integer Programming (MIP): both continuous and discrete variables are used. When all expressions are linear, the framework is referred to as mixed integer linear programming (MILP). When at least one expression is nonlinear, it is referred to as mixed integer nonlinear programming (MINLP). Algorithms for MILPs are the same ones as for IPs. In the case of MINLPs, the main algorithms are branch-and-bound, Generalized Benders Decomposition (GBD) (Geoffrion 1972), Outer-Approximation methods (OA and QOA) (Duran and Grossmann 1986; Su et al. 2018), and the Extended Cutting Plane method (ECP) (Westerlund and Pettersson 1995). MINLPs can at times be linearized via exact linearization or piecewise linear approximations to improve their solvability.

Logic based formulations have also been developed under the framework of Generalized Disjunctive Programming (GDP) (Raman and Grossmann 1994). The GDP formulation is given in (**2**), where c_k is a scalar fixed cost for disjunction k, f is a single-valued function, $g(x) \leq 0$ represents the set of common constraints among scenarios. The OR operator (∨) is used to select amongst a set of alternatives J_k in the set of disjunctions K. When a given alternative is selected, the respective Boolean variable Y is $True$ and activates the constraints of the form $r_{j,k}(x) \leq 0$ and sets the fixed cost to $\gamma_{j,k}$. The vector-valued Boolean function $\Omega(Y)$ is used to incorporate additional logical expressions, which must be $True$ for the solution to be feasible.

$$\begin{aligned}
&\min_{x,Y} \sum_k c_k + f(x) \\
&s.t. \quad g(x) \leq 0 \\
&\qquad \bigvee_{j \in J_k} \begin{bmatrix} Y_{j,k} \\ r_{j,k}(x) \leq 0 \\ c_k = \gamma_{j,k} \end{bmatrix} \quad \forall k \in K \\
&\qquad \Omega(Y) = True \\
&\qquad x \in \mathbb{R}^m
\end{aligned} \tag{2}$$

$$Y_{j,k} \in \{True, False\}$$

The GDP formulation can be reformulated into 0-1 MILP/MINLP problems. In the process, Boolean variables are translated into binary variables. The two main reformulation techniques are the Big-M method and the Hull Reformulation method (Grossmann and Trespalacios 2013). There is a tradeoff between the two in terms of model complexity and model tightness, with the latter resulting in tighter, but more complex models.

Constraint programming (CP) (Hooker and van Hoeve 2018) is a logic-based framework that can be applied to optimization. It is well suited for scheduling problems in which resources are limited and relies on an efficient method for finding feasible solutions via a technique called constraint propagation. Hybrid CP/MILP approaches have also been used to combine the advantages of both methods (Jain and Grossmann 2001; Maravelias and Grossmann 2004). For instance, CP can be used for the sequencing constraints and MILP can be used for the resource assignment constraints. This technique has promising synergy that can significantly improve solution times.

Optimizing under uncertainty plays an important role in industrial applications, in which many different types of uncertainties can be encountered (Sahinidis 2004). Uncertainties can be classified as exogenous or endogenous, depending on what triggers the realization or disclosure of the uncertain parameter values (Jonsbråten 1998). When the triggering is external to the decision maker (e.g. future demand for a product), the uncertainty is termed exogenous, and when it is triggered by the decision maker's choices (e.g. oil field size, which can only be known after drilling and producing), it is termed endogenous. The three main approaches to optimization under uncertainty are Stochastic Programming (Birge and Louveaux 2011), Robust Optimization (Bertsimas et al. 2011), and Flexibility Analysis (Grossmann et al. 1983).

The most common stochastic programming (SP) approach is the two-stage formulation, which is presented in (**3**). The objective function in stochastic programming is an expectation of f given the uncertain parameter ξ, which has a discretized probability distribution. The two-stage formulation separates the here-and-now decisions (x; stage 1) from the wait-and-see decisions (y; stage 2). The latter are recourse decisions that are made in response to a scenario s. A scenario is a state that arises from one of the possible realizations of the uncertain parameters. The formulation can be extended to multi-stage scenarios. Multi-stage scenarios are often represented with a scenario tree as the one shown in **Figure 2** for a three-stage stochastic program under exogenous uncertainty with two realizations (high and low) for the uncertain parameter ξ in each stage. Nodes represent the states of the system at each period and arcs represent transitions from one period to the next.

$$\begin{aligned} \min_{x,y} \quad & \sum_{s \in S} p_s \cdot f(x, y_s, \xi_s) \\ s.t. \quad & g(x, y, \xi) \leq 0 \\ & x \in X \\ & y \in Y \end{aligned} \tag{3}$$

Two important metrics are typically associated with the use of stochastic programming: EVPI (expected value of perfect information) and VSS (value of the stochastic solution). The EVPI quantifies the improvement that is possible if uncertainties are replaced with perfect information. This gives an indication of how valuable it would be to reduce uncertainties by improving forecasting accuracy, for instance. On the other hand, the VSS quantifies the added value of using stochastic programming relative to the deterministic optimization counterpart. These metrics are typically applied to two-stage problems, but can be extended to multi-stage problems as discussed in Escudero, *et al.* (2007).

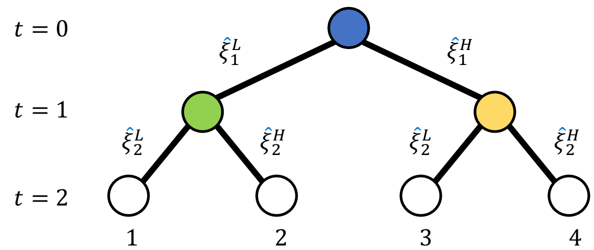

Figure 2. Sample scenario tree for a three-stage stochastic program with exogenous uncertainty

Robust optimization (RO) takes a different approach to uncertainty. Rather than optimizing over possible scenarios given uncertain parameter probability distributions, the focus is on optimizing over a deterministic uncertainty set to guarantee feasibility over all points in the set. The problems can be formulated so that the degree of conservatism is customizable (Bertsimas and Sim 2003). The general formulation for RO is given in (**4**). This formulation is aimed at finding fixed operating variables x that minimize the maximal value of the constraint system under the uncertainty set W. This ensures the solution is feasible for all uncertain points since it is feasible for the worst-case uncertainties in W.

$$\min_{x \in X} \max_{w \in W} \max_{j \in J} f_j(x, w) \tag{4}$$

Extensions to the classical RO approach are Adjustable Robust Optimization (ARO) and Affinely Adjustable Robust Optimization (AARO) (Ben-Tal et al. 2004). In these formulations, the operating variables are a function of the uncertain parameters, meaning $x = x(w)$. In AARO, the relationship between the uncertain parameters and the operating variables is linear, $x = p + Qw$. These approaches have the advantage of increased flexibility in the formulations for more realistic optimization.

Another approach to optimizing over an uncertain set is that of Flexibility Analysis (FA) (Grossmann et al. 1983, 2014), which uses an alternate sequence of optimization operators than that of RO. (**5**) provides the general formulation for FA, which finds the worst parameter w by maximizing over the uncertainty set W, given that the operating variables x are adjusted for each parameter w to minimize the largest constraint in the system. For linear models, FA problems are translated into MILPs, whereas AARO problems are translated into LPs. Although FA is computationally more expensive given its more general treatment of the operating variables, requiring the use of binary variables in its reformulation as an MILP, it provides solutions that are feasible and more rigorous in the uncertainty set when compared to AARO (Zhang et al. 2016). Thus, FA can find better solutions than those proposed by AARO.

$$\max_{w \in W} \min_{x \in X} \max_{j \in J} f_j(x, w) \tag{5}$$

4. Industrial Examples

4.1. Upstream Oil & Gas

According to a market research report by IBISWorld (Mieles 2020), the Oil & Gas E&P (Exploration and Production) industry generated $3.3 trillion USD in revenue in 2019. Of that revenue, roughly 75% came from oil and 25% from gas. The industry as a whole is very capital intensive with a 4:1 capital investment to labor costs ratio. CAPEX (capital expense) for production facilities can be on the order of billions of dollars in the case of offshore facilities. Optimization in this industry can generate significant value, as even small percentages in cost reduction or revenue increase can amount to millions of dollars. As a result, several studies have focused on the optimization of both offshore and onshore facilities. Industrial optimization examples in each of these areas are presented in this section.

4.1.1. Offshore deep-water oilfield development

An application of mathematical programming to plan the optimal development of deep-water oil fields is presented in Gupta and Grossmann (2012). A multiperiod nonconvex MINLP model is used to plan the development and production of multiple oil fields. The model accounts for simplified reservoir models and multicomponent (oil, gas, and water) systems. Key decisions the offshore development planning model belong to the following areas,

- Installation and expansion timing for FPSO (floating production and storage) units,
- FPSO unit capacities,
- FPSO connections to the oil fields,
- number of wells to drill in each field,
- oil and gas production rates at each field.

The objective of the model is to maximize the NPV (net present value) of the offshore development project. High order polynomials for the reservoir profiles in terms of cumulative water and cumulative gas production are used to avoid the bilinear terms resulting from using water-oil ratios or gas-oil ratios. The model can also be reformulated as an MILP by using exact and piecewise linearization techniques to find the global optimum of the approximated problem. **Figure 3** illustrates a piecewise linearization of a nonlinear oil delivery profile.

A case study for the above model is presented for a project with a 20-year horizon, 10 oil fields, 3 FPSOs, 23 wells, 3-year lead time for FPSO installation, and 1-year lead time for facility expansion. The MINLP model has approximately 500 binary variables, 5,700 continuous variables, and 9,900 constraints. It is solved in 67 seconds using DICOPT 2x-C on an Intel Core i7 with 4 GB of RAM to yield an optimal NPV of $30.95 billion USD. The reformulated MILP has approximately 1,600 binary variables, 12,000 continuous variables, and 17,000 constraints and requires a considerably longer computational time (approx. 4.5 hours) to find a global optimum of $30.99 billion USD. Connection schedules and production rates are shown in **Figure 4** and **Figure 5**. The three FPSOs are installed within the first two years and production begins in the end of year three (beginning of year four), with additional field connections scheduled for the following three years.

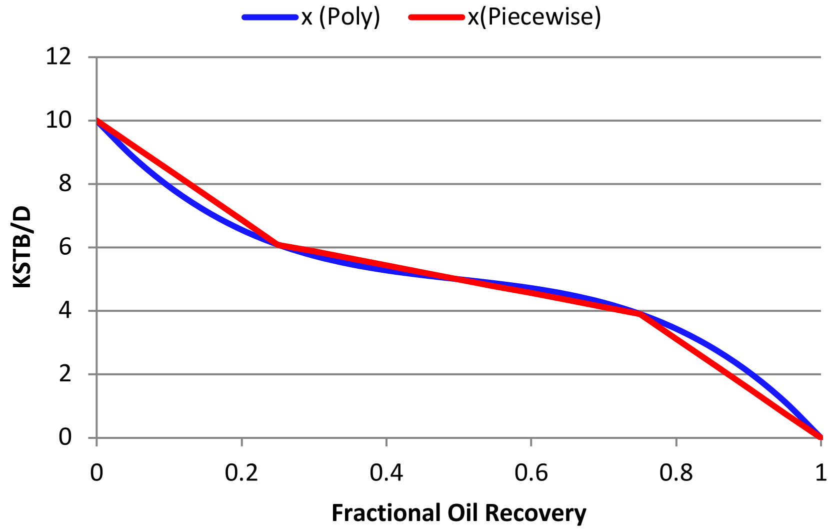

Figure 3. Sample piecewise linearization for oil deliverability profiles (Gupta and Grossmann 2012)

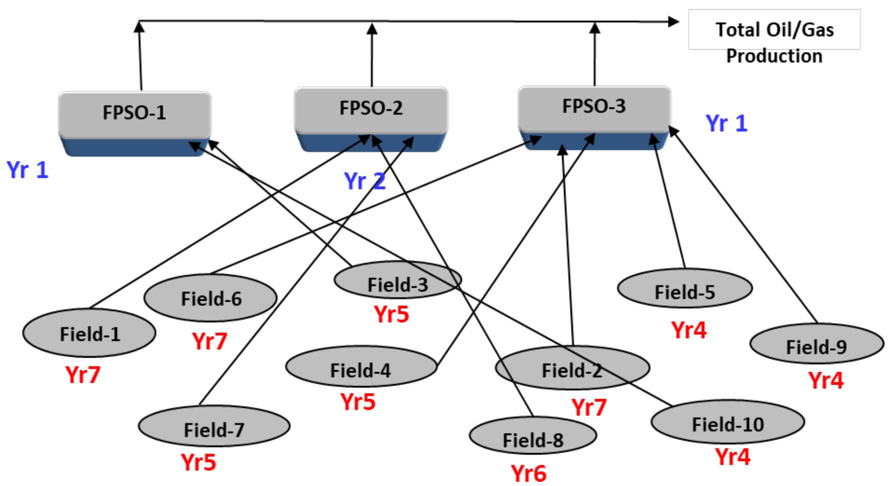

Figure 4. Installation plan for deep-water case study (Gupta and Grossmann 2012)

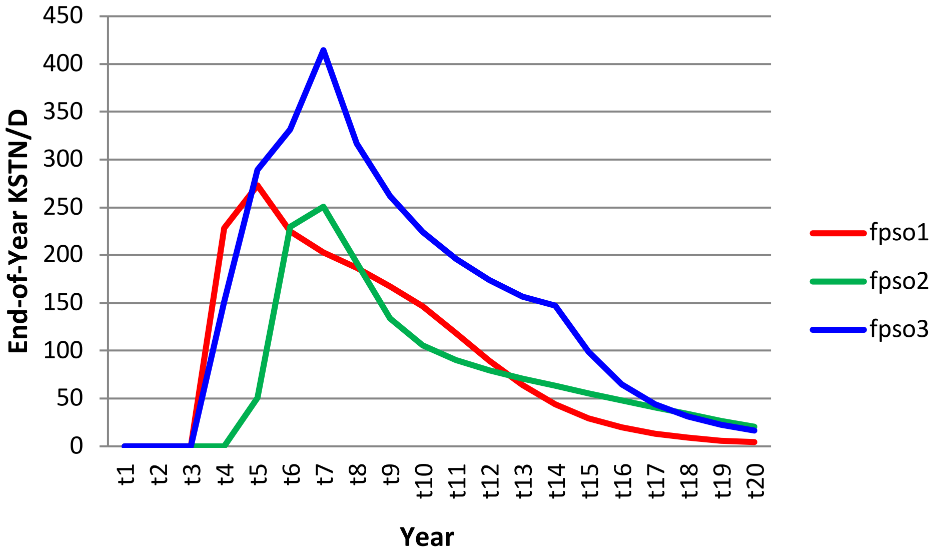

Figure 5. Oil production rates for deep-water case study (Gupta and Grossmann 2012)

The 2012 deterministic model discussed above has been extended to a multi-stage stochastic model that accounts for 1) endogenous uncertainties in the oil field parameters and 2) fiscal contracts involving taxation and royalties (Gupta and Grossmann 2014). **Figure 6** displays the predicted revenue distribution included in the model. Langrangean decomposition is used to parallelize and improve the computational performance during solution time. For a project with 3 fields and three FPSOs, studies show the benefits of using decomposition techniques for solving stochastic programs. When 4 scenarios involving uncertainties in the oil field size, oil deliverability, water-oil ratio, and gas-oil ratio are included in the project, the full-space model is solved to optimality using CPLEX 12.2 in under 3 hours, yielding an expected NPV of $12 billion. Decomposition yields a solution that is only 0.5% below the optimum and has an optimality gap of less than 2%. However, the solution times for the decomposed model are 7.3 and 4.3 minutes for the sequential and parallel implementations, respectively. This is a significant speedup of 2 orders of magnitude.

Another instance that includes uncertainty in the oil field size (4 scenarios) and accounts for progressive production sharing agreements shows that the sequential and parallel decomposition implementations find a solution of $3 billion with an optimality gap of 0.7% in only 2 hours and 1 hour, respectively. On the other hand, the full-space model times out after 10 hours with a 21% optimality gap and a solution that is 2.3% below the solution obtained via decomposition. Larger instances with 5 oil fields and up to 8 scenarios show that even though decomposition strategies become more computationally expensive, they find better solutions with tighter bounds much faster than the full-space models.

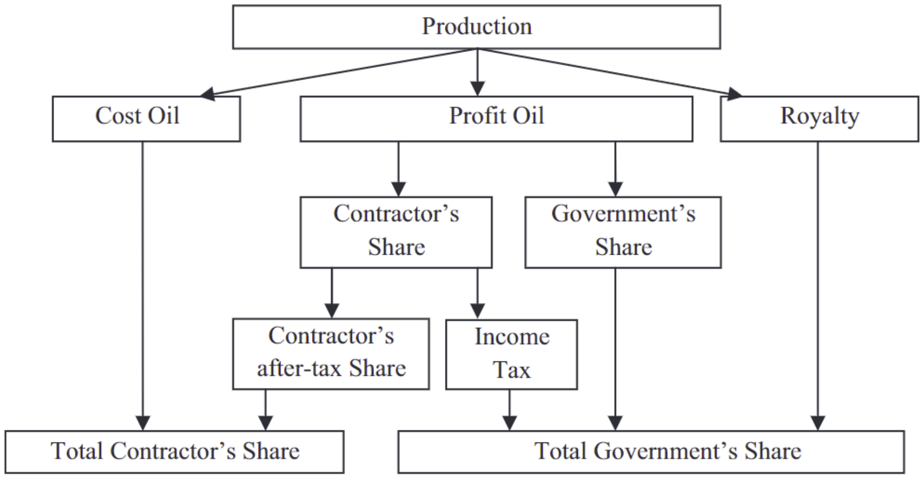

Figure 6. Revenue flows in typical production sharing agreements (Gupta and Grossmann 2014)

4.1.2. Onshore shale gas development

A multiperiod planning MINLP model for shale gas development projects is presented in Drouven and Grossmann (2016), which extends the work by Cafaro and Grossmann (2014). The model uses a shale gas development superstructure and optimizes decisions in the following areas,

- Selection of well pad locations,
- Timing of well pad construction,
- Selection of number of wells to drill and their location,
- Timing of drilling operations,
- Allocation of available drilling rigs,
- Selection of locations for processing plants and compressor stations,
- Allocation of available compressors, and
- Layout and design of pipelines.

Figure 7 illustrates the superstructure for a greenfield shale gas development case study with a 10-year planning horizon, 10 candidate well pads in three pad clusters, 1 processing plant, 1 compressor station, 1 freshwater source, and varying well compositions by well clusters. The resulting MINLP model consists of 13,000 constraints, 10,000 bilinear terms, and 25,000 binary variables. The model was optimized in approximately 1.5 hours to yield an NPV of $214 million USD, which is a 2.6 times higher NPV than the historic development strategy used for that project. This NPV was achieved by improving equipment utilization and scheduling return-to-pad operations, which incurred 14% more development expenses, but required 23% less wells to be drilled. The optimal structure and operating schedules are given in **Figure 8** and **Figure 9**, respectively.

In the work by Cafaro, *et al.* (2016), planning of shale gas refracturing is proposed via two main approaches, 1) a continuous-time NLP model based on productivity decline forecasts, and 2) a discrete-time MILP model that explicitly accounts for multiple refractures. The MILP model is obtained via reformulation of a GDP model, and takes three different forms depending on the reformulation approach (big-M reformulation, standard hull reformulation, and compact hull reformulation). The model is coupled with multiple price forecasting models and a reservoir simulation model with real data. The model sizes are given in **Table 1** below. Although the hull reformulations result in significantly larger models, the model complexity is paid off with the superior computational performance observed. The reduced model size of the compact hull reformulation allows it to outperform the standard hull reformulation, taking less than half of the time required to solve the latter. For the real case study, the solutions find significant increases in the development NPV and well recovery. Well recoveries are increased by up to 25% and profits by hundreds of thousands of dollars when using the optimized plan.

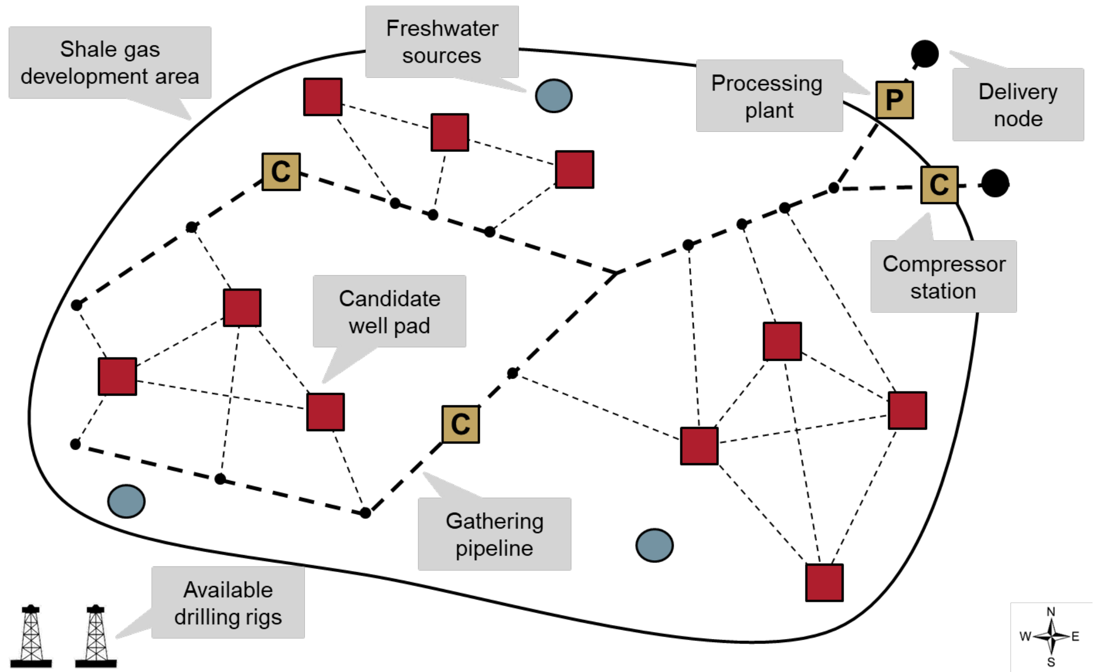

Figure 7. Case study shale gas development superstructure (Drouven and Grossmann 2016)

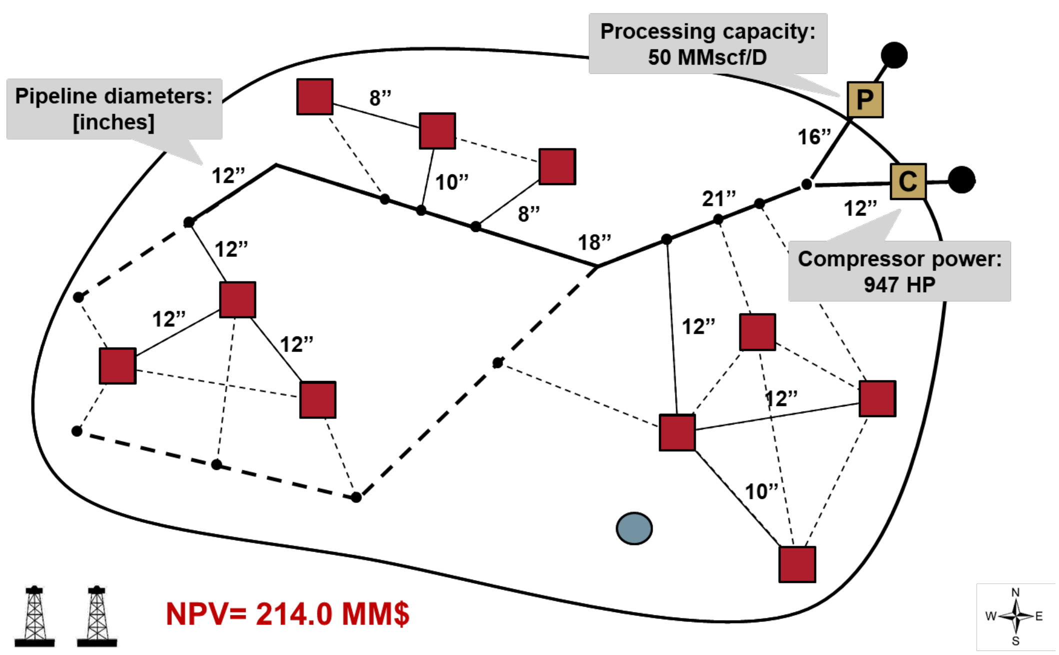

Figure 8. Optimal shale gas structure (Drouven and Grossmann 2016)

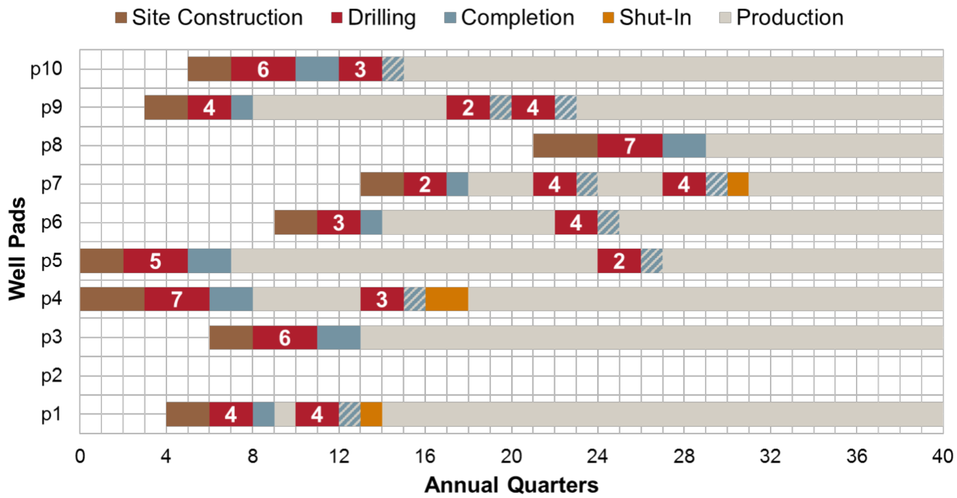

Figure 9. Optimal shale gas development schedule with number of wells drilled indicated within the drilling tasks (Drouven and Grossmann 2016)

Table 1. Model sizes and run time (using Gurobi 5.6.2) for the big-M formulation (BMF), standard hull reformulation (SHR), and compact hull reformulation (CHR) MILP models (Cafaro et al. 2016).

	BMF	SHR	CHR
Binary Variables	240	360	360
Continuous Variables	481	44,161	22,381
Constraints	15,603	89,163	67,383
Nodes Explored	7,786	0	0
Solution Time (s)	255	22	9

4.2. Multiperiod Blending

Blending operations are key in many industries, such as the downstream petrochemicals, food, and pharmaceuticals industries, where most product recipes contain one or more blending steps. **Figure 10** shows a sample configuration for a blending problem consisting of supply, blending, and demand tanks. From a mathematical programming standpoint, blending problems are difficult to solve due to bilinear terms that give rise to nonconvex MINLPs. Different approaches have been taken to improve the solvability of these models. In Lotero, *et al.* (2016), an alternate formulation with redundant constraints is used to tighten and improve the model relaxations. The authors also present a bilevel decomposition algorithm that outperforms state of the art general purpose solvers. In the decomposition algorithm, a master MILP is solved to fix binary variables in a subproblem containing a reduced MINLP. **Figure 11** shows the proposed decomposition algorithm and **Figure 12** compares the performance of the proposed algorithm with the SCIP solver. The decomposition approach finds the global optimum in a reasonable amount of time (approximately 20 minutes on average for the 45 instances studied), whereas the general purpose SCIP solver, times out with a large optimality gap. The instances studied were for 6 and 8 time periods and 1 to 10 stream specifications, resulting in models with 240-320 binary variables, 128-1,760 bilinear terms, 552-1,312 continuous variables, and 984-3,616 constraints.

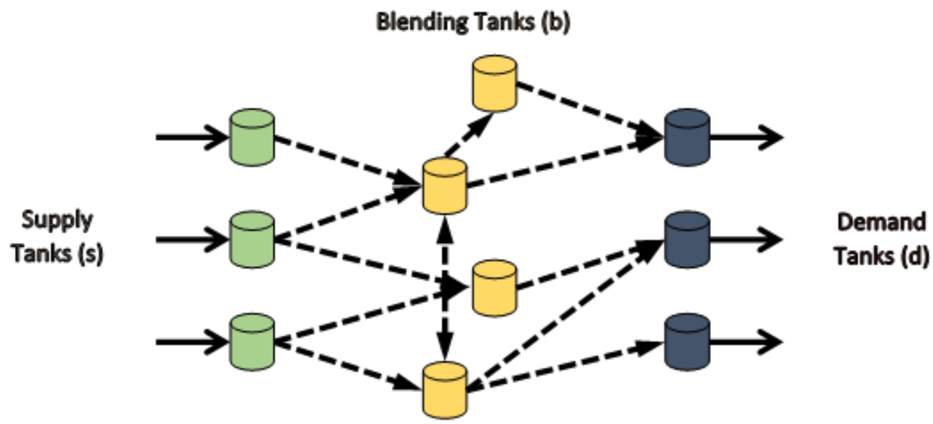

Figure 10. Sample schematic for blending problem (Lotero et al. 2016)

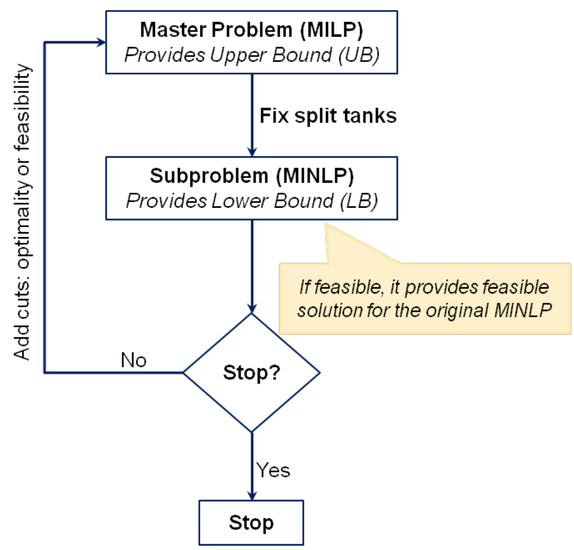

Figure 11. Bilevel decomposition algorithm for multiperiod blending problem (Lotero et al. 2016)

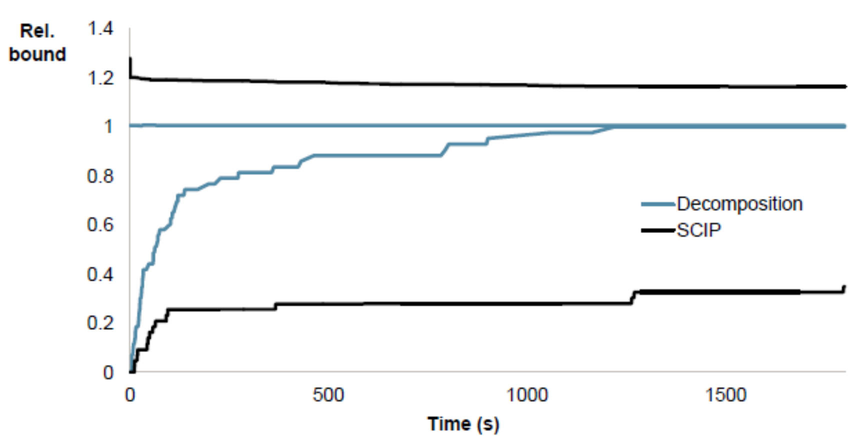

Figure 12. 43-instance average relative upper and lower bounds for decomposition algorithm and SCIP solver (Lotero et al. 2016)

4.3. Processing Plant Designs

MINLP has been applied to the optimization of biological and chemical processing plants. One example is the optimization of a natural gas plant design presented in Caballero, *et al.* (2007). This work integrates GDP with the commercial process simulator HYSYS to find the optimal equipment types and utility selections for the plant. The reformulated MINLP is coupled to a HYSYS flowsheet and has 38 explicit nonlinear constraints, 5 linear constraints, 16 binary variables, 19 external variables (7 are flowsheet specifications), and 40 implicit blocks of equations (for cost, sizing, and correlations). The two algorithms applied are an LP-NLP Branch-and-bound and Outer approximation. The LP-NLP BB algorithm solves 23 LP nodes and 2 NLP subproblems, requiring 300 seconds to find the minimum cost design of $117 thousand/year. The OA approach performs 4 major iterations and solves 3 NLP subproblems in 708 seconds. The optimal design with equipment selections and utility specifications is shown in **Figure 13**.

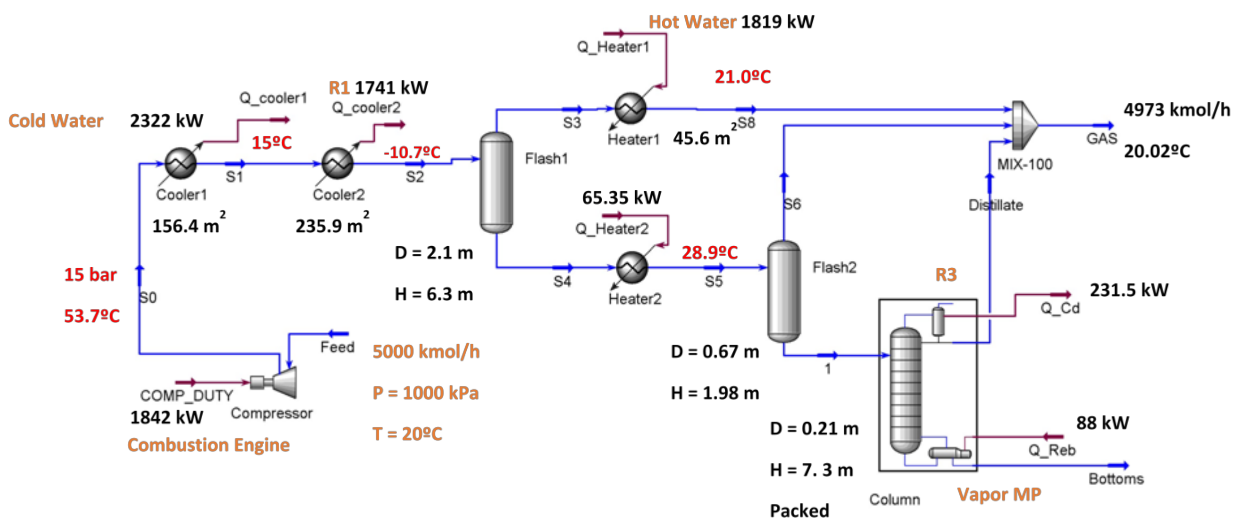

Figure 13. Optimal natural gas plant design (Caballero et al. 2007)

Another example is the economic evaluation and design of a plant for bioethanol and biodiesel synthesis presented in Martín and Grossmann (2015). The work uses MINLP for superstructure optimization of a plant with several alternative biochemical pathways. The model includes two biomass pre-treatment alternatives, mainly ammonia fiber explosion (AFEX) and dilute acid pretreatment. Pre-treatment is followed by hydrolysis, from which the intermediate material can either be fermented and purified to produce biodiesel or bioethanol. An additional feature of the model is that it accounts for heat integration for the plant by performing a heat exchanger network synthesis simultaneously during the optimization. From the data used in the model, the production of biodiesel is determined to be economically infeasible. The model allows to perform a sensitivity study to understand the technological improvements required in terms of conversion ratios (greater than 50%) for biodiesel to become economically feasible.

In another study by Martín and Grossmann (2011), superstructure optimization with MINLP is used to design a lignocellulosic ethanol process via gasification. The superstructure includes alternate technological pathways for the different stages of bioethanol production as depicted in **Figure 14**. The MINLP superstructure can be decomposed into 8 subproblems that can be solved as NLPs as shown in **Figure 15**. Within each subproblem, the following subsystems are linked sequentially: syngas composition adjustment, sour gas removal, and ethanol purification. MINOS, KNITRO, and CONOPT3 (NLP solvers) are used to initialize the subsystems. Heat integration using the SYNHEAT heat integration software is then included on each of the subproblems to design an energetically optimal system. Multi-effect distillation is used to strengthen the heat integration in the final purification step. The optimal design results in a production cost of $1.04/gal of ethanol and involves high pressure gasification, steam reforming, PSA H_2, PSA/MEA, catalytic reactor, and direct distillation. The cost is further reduced with H_2 byproduct credits to $0.41/gal. These results show potential achieved through optimization when compared to the other cost evaluations in literature, which range from $1-2/gal.

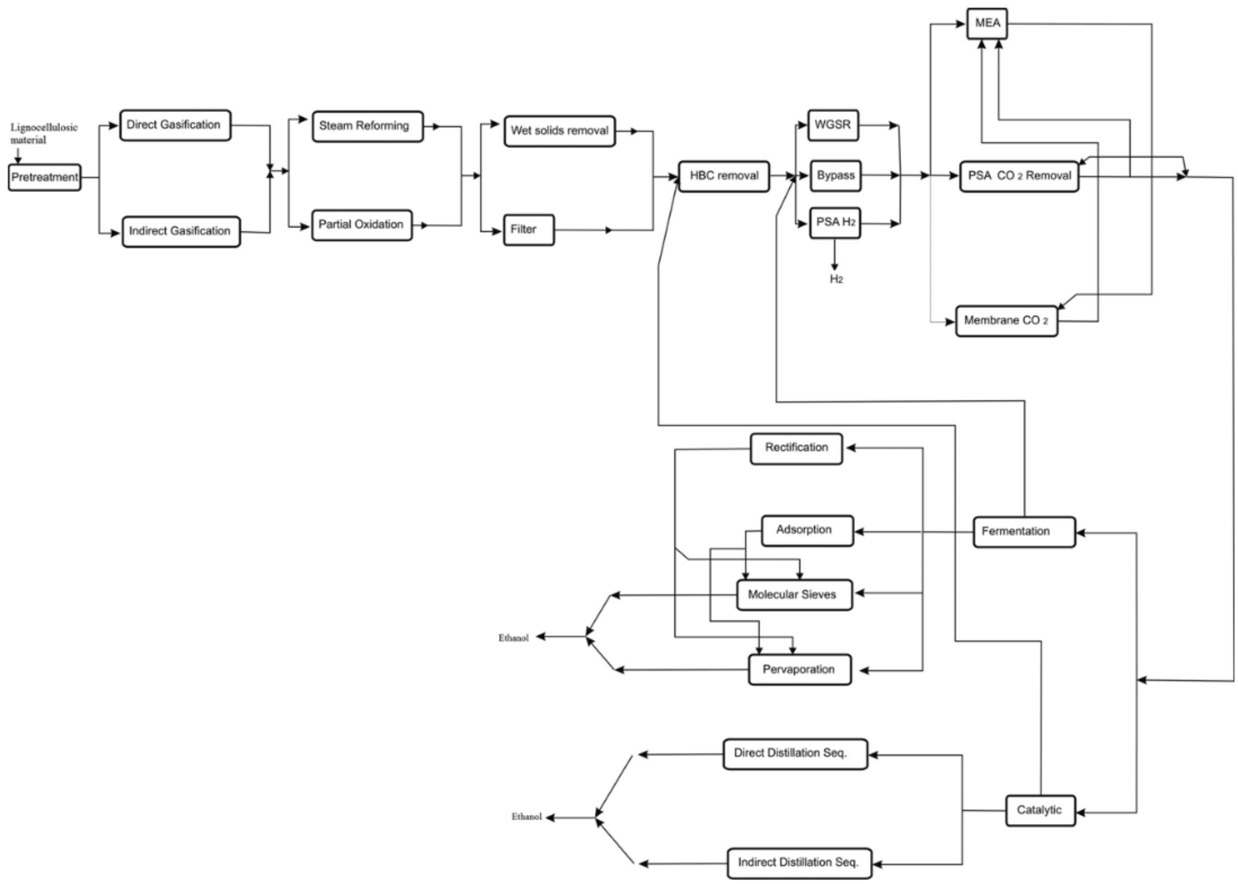

Figure 14. Technological pathways for bioethanol production (Martín and Grossmann 2011)

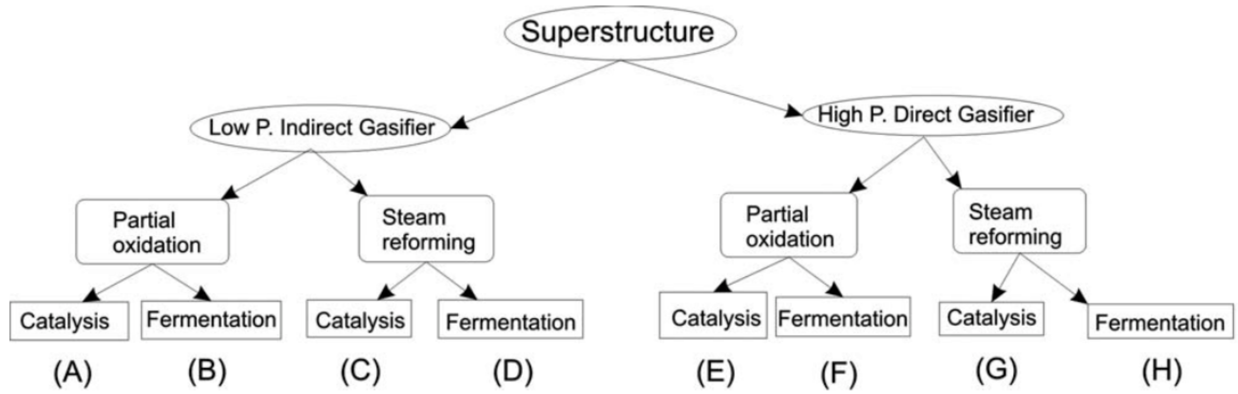

Figure 15. Superstructure subproblems for bioethanol production (Martín and Grossmann 2011)

4.4. Facility Network Design

Lara, *et al.* (2019) present a novel algorithm for planning and designing manufacturing networks that takes into account the tradeoffs between the decision to build centralized facilities versus the decision to build distributed facilities. The tradeoff is of economies of scale versus transportation costs, which play key roles in the profitability of manufacturing networks. The model used is a multi-period GDP extension of the Capacitated Multi-facility Weber Problem that is reformulated as a non-convex MINLP and solved with an accelerated bilevel decomposition algorithm that provides tight bounds and outperforms the commercial global optimizers BARON, SCIP, and ANTIGONE as shown in **Figure 16**. The model uses the locations of customers and suppliers and iteratively refines the grid partitioning of the two-dimensional geographical space to find the optimal facility locations and make the optimal facility type decisions to meet location specific customer demand and minimize costs.

An application is presented in the design of a bioethanol supply chain with 10 suppliers, 10 markets, 10 potential distributed facilities, and 2 potential centralized facilities. The model has 1,320 binary variables, 1,545 continuous variables, and 3,457 constraints. Three iterations of the accelerated bilevel decomposition algorithm during 6 hours were required to solve the problem to a 2% optimality gap with a net present cost of approximately $2 billion. The proposed algorithm proved superior to BARON, which still had an optimality gap of 68% after 10 hours of run time. The optimal supply chain design is illustrated in **Figure 17**. The investment schedule includes building 10 distributed facilities in the first year and a single centralized facility in the second year.

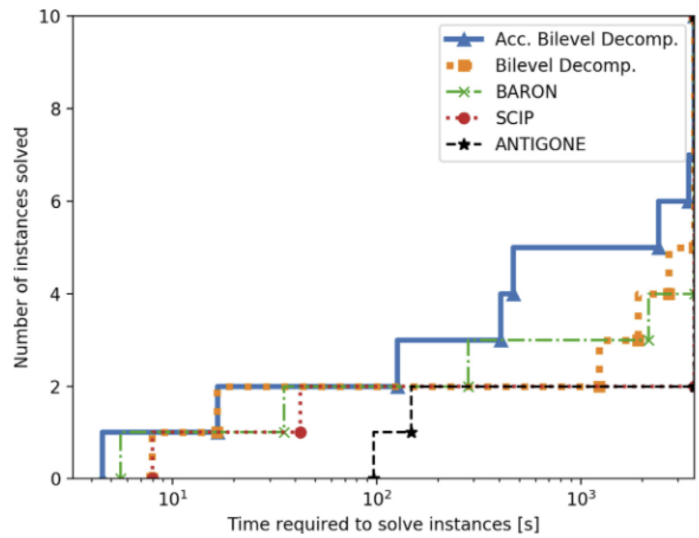

Figure 16. Performance profiles for the standard and accelerated bilevel decomposition algorithm in Lara, et al. (2018, 2019) and the commercial solvers BARON, SCIP, and ANTIGONE

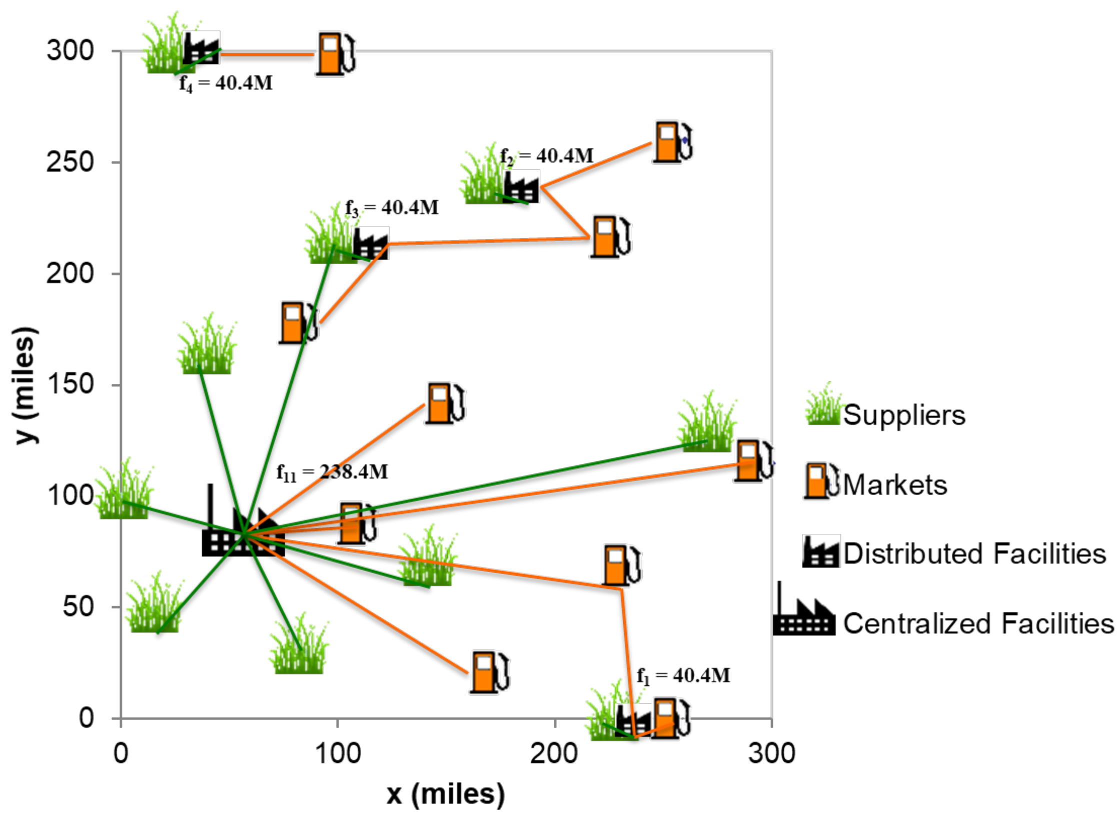

Figure 17. Optimal supply chain network structure for the biomass case study

4.5. Water Network Design

Global optimization techniques are important in solving water network design problems that require water treatment facilities for water leaving processing facilities, a common requirement in many industries. This problem is formulated in Karuppiah and Grossmann (2006) as a superstructure optimization with a nonconvex NLP or a nonconvex GDP in which all possible interconnections between water-using process equipment and treatment units are considered so as to account for reuse and recycle of water. Techniques such as convex envelopes, explicit tight variable bounds inferred from the superstructure, and novel bound strengthening cuts based on flow balances are used in a spatial branch and contract algorithm to solve this problem efficiently. The strengthening cuts also prove very advantageous when used with BARON, solving problems that were virtually unsolvable by BARON. As an example, in one of the instances studied, no solution was found after more than 10 hours of solution time. When the strengthening cut was added to BARON, the problem solved in 1.06 seconds.

The work by Karuppiah and Grossmann (2006) is continued in that of Ahmetović and Grossmann (2011). An industrial water network case study is depicted with the superstructure in **Figure 18**. The notation in this superstructure is as follows, nodes with *PU* are processing units (5 in total), nodes with *TU* are treatment units (3 in total), red triangle nodes are mixers, and blue triangle nodes are splitters. The study quantifies the tradeoff between investment cost and the network complexity. A pareto plot of this tradeoff is shown in **Figure 19**. For all the points in this front, the water consumption was 40 t/h, representing a reduction of more than 85% in the standard water consumption at the plant. The simplest network, with 13 removable connections is depicted in **Figure 20**. The model for this instance has 72 binary variables, 233 continuous variables, and 251 constraints. Solution time in BARON is under 200 seconds with a 1% optimality gap stopping criteria.

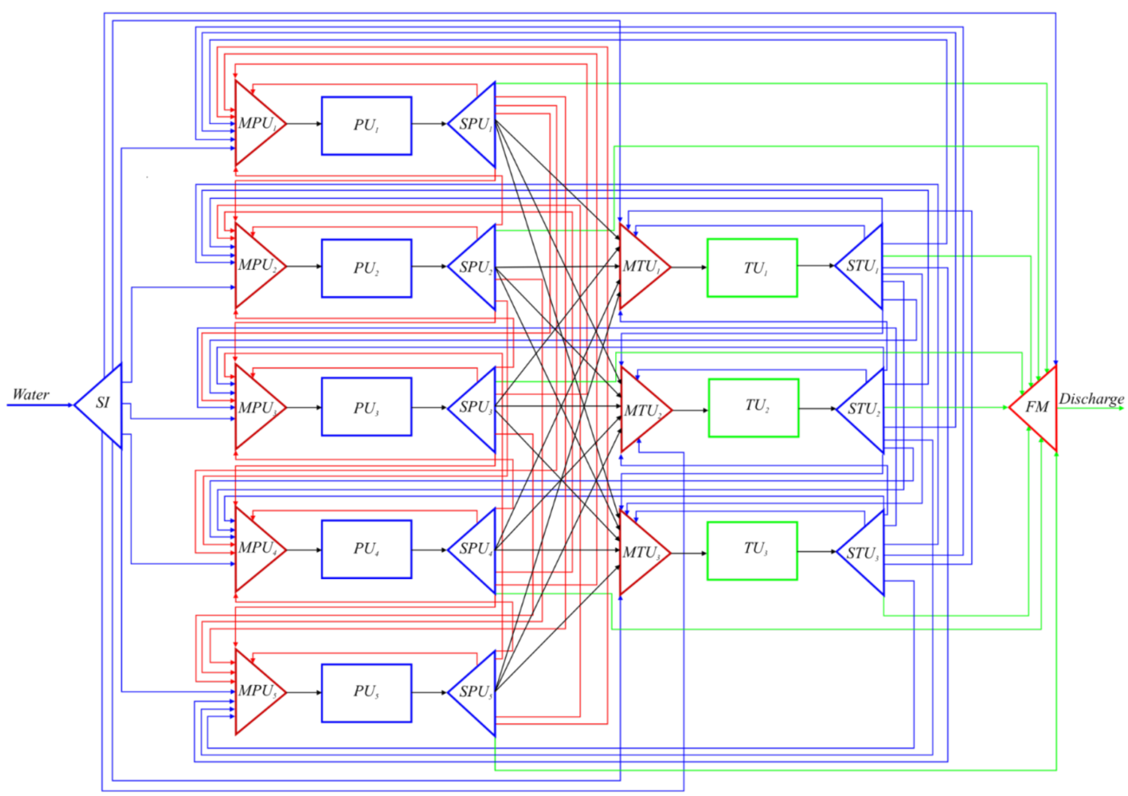

Figure 18. Sample superstructure for facility water network (Ahmetović et al. 2017)

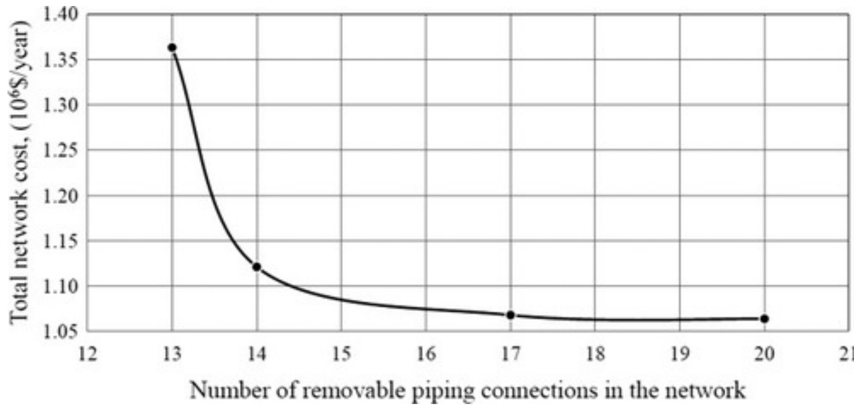

Figure 19. Pareto-optimal front for the water network design case study (Ahmetović and Grossmann 2011)

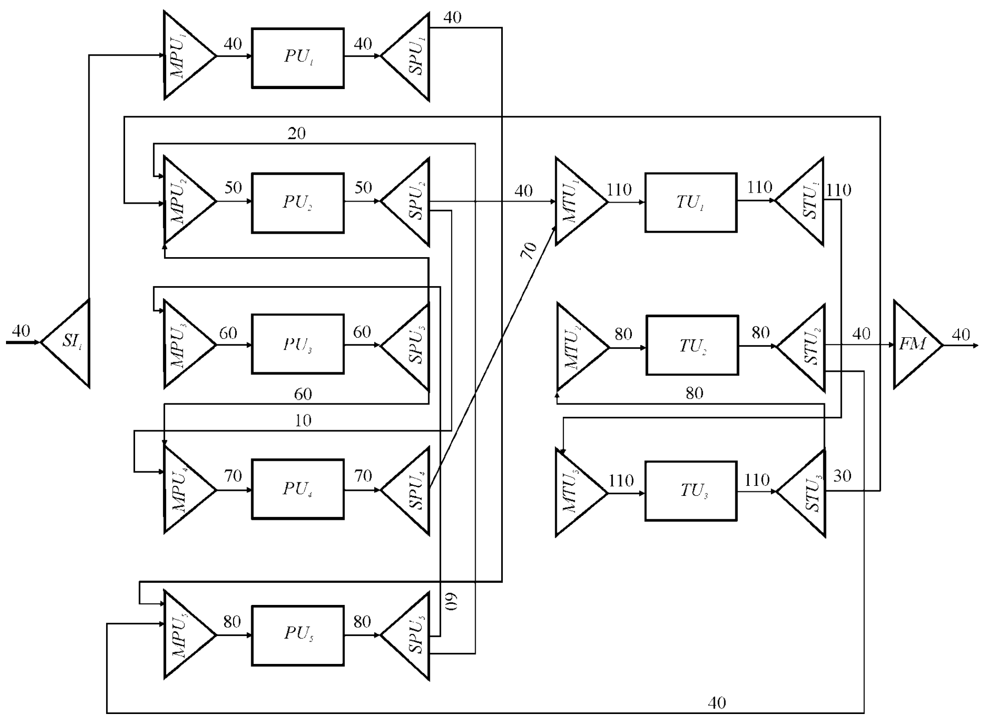

Figure 20. Simplest configuration on the pareto front for the optimal water network design (Ahmetović and Grossmann 2011)

Other works have also shown that these design problems can be solved with increased levels of detail in the process models used. Yang, *et al.* (2014) introduce shortcut models for the treatment units rather than using simple fixed contaminant removal models. This approach makes optimization results more realistic and applicable. The shortcut models used account for mass transfer of contaminants in the treatment units. This allows the optimization models to represent the connection between treatment costs and removal efficiencies, providing more realistic solutions. Other extensions include the use of nonlinear cost functions for operating and investment costs of treatment units, and addressing uncertainty in the contaminant loads present via worst-case, best-case, and nominal scenarios. The increased complexity of the models is mitigated by using Lagrangean decomposition strategies to solve the problems to global optimality.

4.6. Electricity Market Integration

Cryogenic energy storage (CES) technology makes it possible for chemical industries to integrate their processes with the energy market. In a work done by Zhang, *et al.* (2015), an optimization model is proposed to integrate the operations of an air separation unit (ASU) with the energy market via CES. The process, which is illustrated in **Figure 21**, allows for an ASU to produce surplus liquid nitrogen and oxygen to create a CES inventory that can then be used for one or more of the following alternatives, 1) to generate electricity with a gas turbine for internal use, 2) to sell electricity at the spot price on the energy market, or 3) to commit electricity on the reserve market. High electricity spot prices make options 1 and 2 attractive, whereas the fact that revenue from the operating reserve market is created regardless of whether the electricity is actually sold or how much of it is sold makes option 3 attractive. However, option 3 introduces uncertainty that must be properly addressed to avoid severe penalties for not providing the reserve capacity immediately upon request. The uncertainty present here is three-fold: amount, time, and duration of the reserve demand. To properly plan for such uncertainty and capture the benefits of participating in the operating reserve market, adjustable affine robust optimization (AARO) is used on an MILP scheduling model for the integrated ASU/CES system. The model has 2.5 thousand binary variables, 55 thousand continuous variables, and 53 thousand constraints. Solution time with CPLEX 12.5 is 10 minutes with a 1% optimality gap stopping criteria.

The proposed ASU/CES system is tested under varying degrees of conservatism in regard to the operating reserve demand. Even with the highest level of conservatism (assuming that operating reserve can be requested every day), a 5% cost reduction in utilities, especially during peak times, is achieved under the proposed system. For moderate levels of conservatism, the savings are on the order of 9%. **Figure 22** shows the optimal operating schedule for the most conservative case. Another benefit of the integrated ASU/CES system is that of increased plant operation as shown in **Figure 23**.

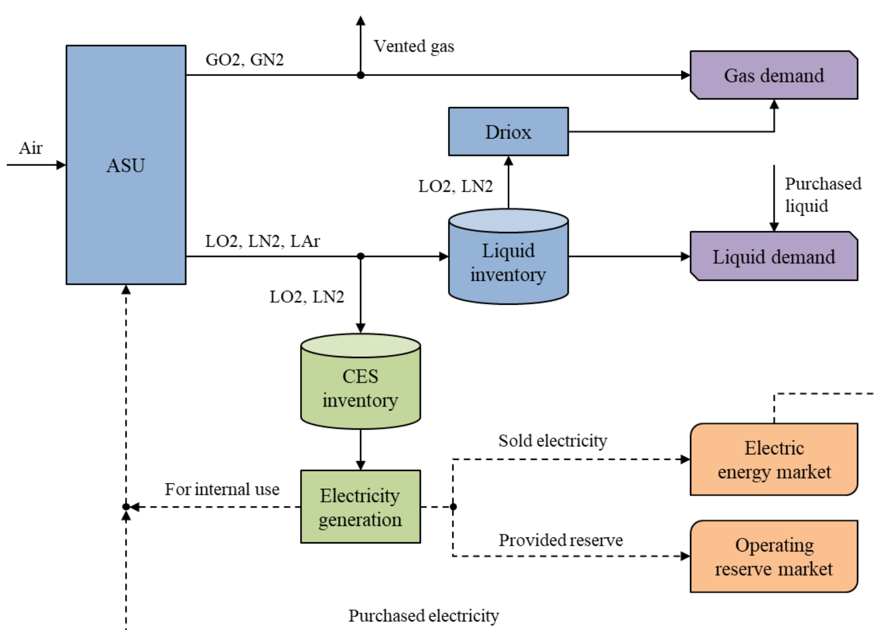

Figure 21. Proposed ASU/CSE system for energy market integration (Zhang et al. 2015)

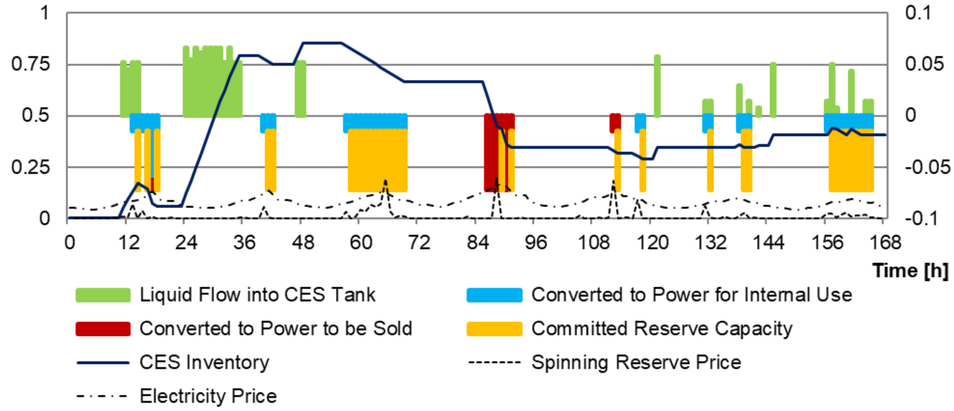

Figure 22. Optimal operating schedule for conservative reserve demand scenario (Zhang et al. 2015)

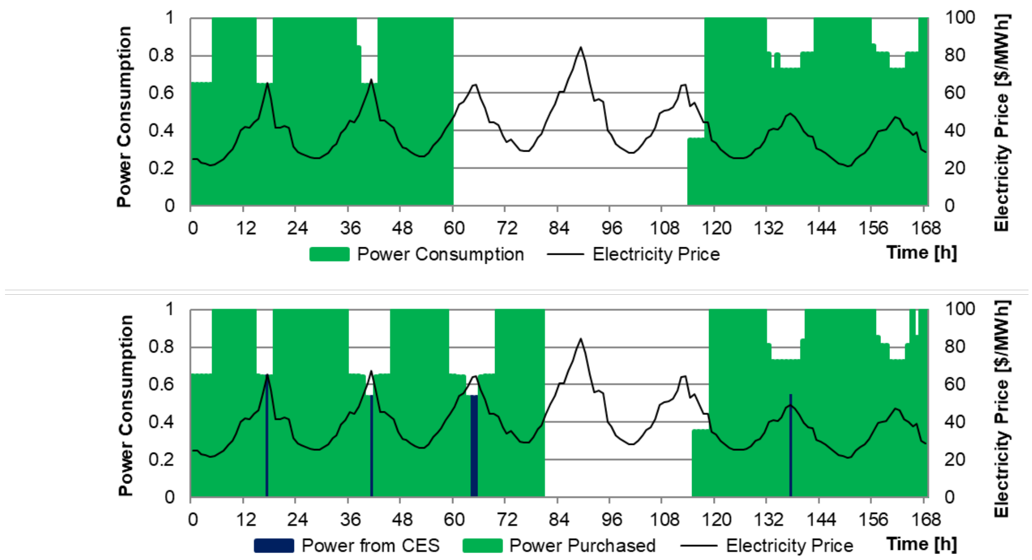

Figure 23. Power consumption and electricity price profiles for the design with no CES capabilities (top) and the design with CES (bottom) (Zhang et al. 2015)

4.7. Reliable Plant Design

In the chemical and manufacturing industries, plant reliability is essential for maintaining competitivity and profitability. However, plant synthesis and optimization approaches often ignore the need for redundant equipment and probabilities of equipment failure. The work by Ye, *et al.* (2018) proposes a model for designing reliable plants that are serial in structure. Options within the superstructure include installation of prioritized redundant equipment with identical characteristics and redundant equipment with varying capacities or features. A geometric distribution is used to model stage availability. Equipment costs in the model include both installation and repair costs. Two formulations are presented with different objectives: 1) profit maximization and 2) plant availability maximization. An advantage of the second formulation is that it can be reformulated as a convex MINLP, whereas the profit maximization formulation is nonconvex. The availability maximization model uses an ϵ-constraint to limit equipment costs. The model facilitates assessing the tradeoffs between plant availability and cost as shown in **Figure 24**. For designs below the pareto curve, it is possible to simultaneously improve availability and reduce cost up until a point on the pareto curve is attained. However, beyond that point, it is not possible to simultaneously improve both objectives. An improvement in one objective, requires a worsening in the other. The only way to improve availability is to increase the upper bound on the equipment cost.

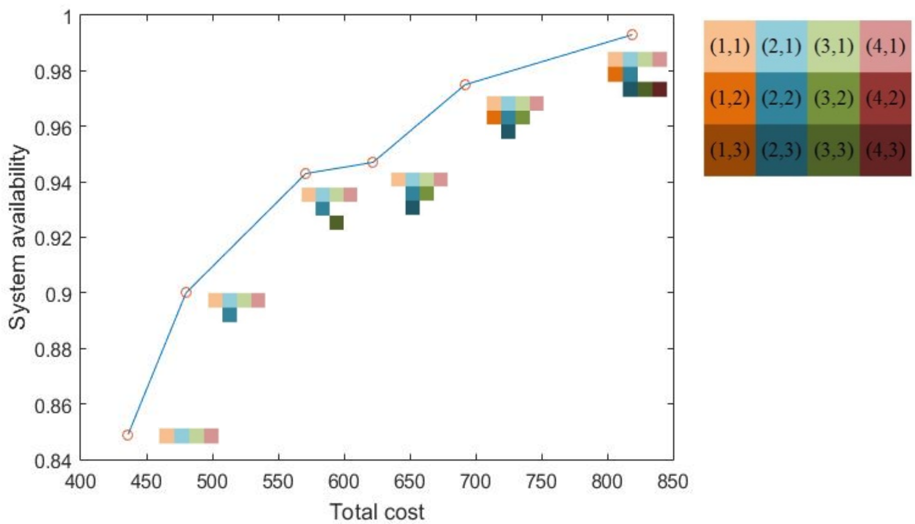

Figure 24. Sample pareto plot of system availability vs total equipment cost for a system with four stages and three potential redundant units per stage (Ye et al. 2018)

Two case studies for the reliable design of a methanol synthesis plant (Türkay and Grossmann 1996) and a toluene hydrodealkylation plant (Kocis and Grossmann 1989) are conducted. The methanol synthesis reliability model consists of 72 binary variables, 451 continuous variables, and 408 constraints. Solution time is 0.45 seconds with DICOPT (CONOPT 3.16D and CPLEX 12.6) to attain an optimal profit of $3.40 million/yr and an availability of 97%. This is an improvement in the optimal design presented in the literature, which ignores potential equipment failures, resulting in a profit of $3.35 million/yr (1.5% lower) and an availability of 92%. The hydrodealkylation model is larger with 400 million design alternatives, 108 binary variables, 955 continuous variables, and 893 constraints, yielding an optimal profit of $3.97 million/yr in 10 seconds of solution time. This solution has a profit that is 4% higher than a naïve design that ignores plant reliability. Availability is increased from 90% to 94% by considering equipment redundancy. The optimal reliable designs for the methanol and hydrodealkylation plants are given in **Figure 25** and **Figure 26**. Reliability optimization allows for increases in both plant reliability and profit in the order of a few percentage points since it mitigates losses due to plant failures.

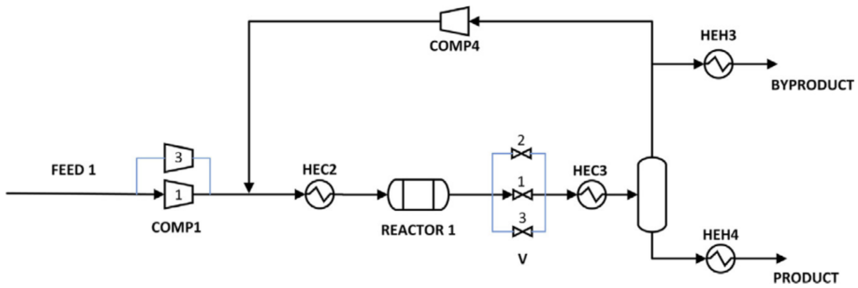

Figure 25. Optimal design for a methanol synthesis plant with redundant units (Türkay and Grossmann 1996; Ye et al. 2018)

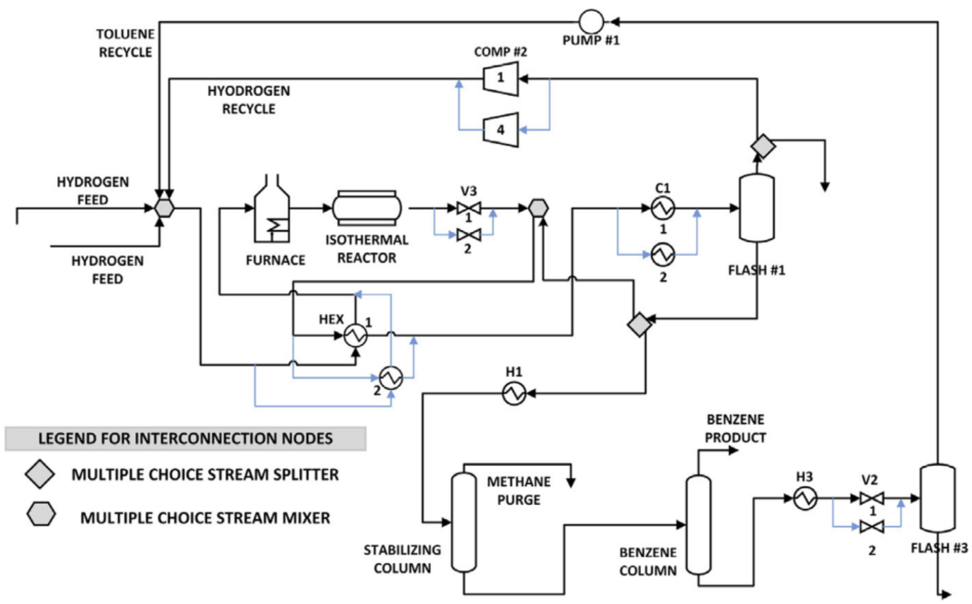

Figure 26. Optimal design for a hydrodealkylation plant with redundant units (Kocis and Grossmann 1989; Ye et al. 2018)

4.8. Resilient Supply Chain Design

Expanding the scope of reliability to the supply chain level, reliability of supply chains in view of disturbances is critical to effective supply chain management. The motivating problem in Garcia-Herreros, *et al.* (2014) is that of a supply chain with one manufacturing facility that produces multiple commodities that are sent to multiple distribution centers to satisfy demands at different customer locations. Potential distribution center locations are preselected. Disturbances in the system occur when disruptions occur at the distribution centers. There is a fixed probability of disruption for each distribution. The key decisions are whether to establish a distribution center at a preselected location and with what capacity to install it. A two-stage stochastic programming model is proposed where the first stage decisions are the distribution center selection and capacity assignments, and the second stage decisions are the assignment of commodity specific customer demands to each available distribution center under each disruption scenario. The model is solved with a strengthened multi-cut Benders decomposition (Birge and Louveaux

1988). Additionally, several techniques are applied to improve the model's solvability. The four main techniques are as follows,

1. Indistinguishability: indistinguishable scenarios are identified as those with disruptions at locations that were not selected. Only one instance is solved for each indistinguishable set.
2. Parallelization: Benders subproblems are parallelized.
3. Relevant scenario selection: scenarios with very low probabilities of occurring are set aside to allow the model to be tractable despite the exponential increase in scenarios as the problem size increases.
4. Bounding excluded scenarios: a procedure for providing bounds on the full space model that accounts for the excluded scenarios after the optimization completes is used.

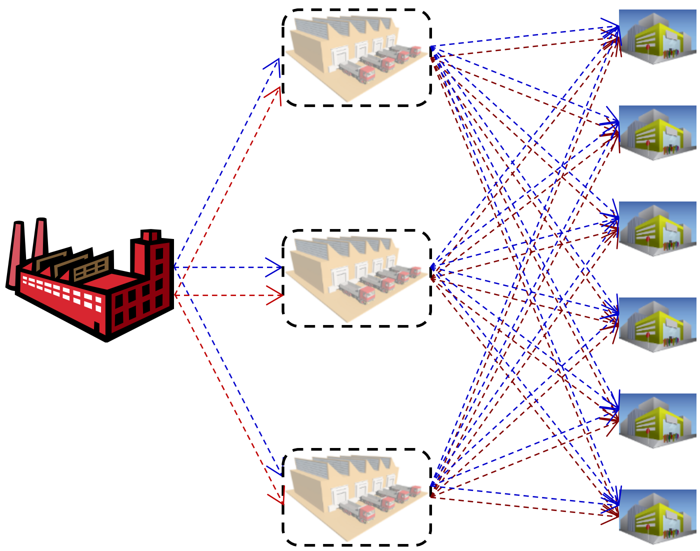

Figure 27. Sample multi-commodity distribution system with 1 plant, 3 distribution centers, and 6 customers (Garcia-Herreros et al. 2014)

The model is applied to an industrial supply chain design problem with 29 candidate distribution centers with disruption probabilities ranging from 0.5% to 3%, 110 customers, and 61 commodities. The total number of scenarios that would need to be considered is $2^{29} \approx 540\, million$. However, using the techniques described previously the problem can be solved in under 5 hours for a reduced problem set with at most 1 disruption at a time and 30 scenarios that covers 85% of the total probability of scenarios. The model size for this instance is of 29 binary variables, 250 thousand continuous variables, and 300 thousand constraints. Increasing the coverage to 98.5% of the total probability of scenarios (436 scenarios in the set), by allowing up to 2 simultaneous disruptions, increases the run time to around 5 days with less than a 1% optimality gap. The model size here is 29 binary variables, 3.6 million continuous variables, and 4.4. million constraints. In this case, the scenario set is within the full space bounds, which is not the case in the deterministic problem nor in the 30-scenario set problem.

5. Conclusions

An overview of continuous and discrete optimization models has been presented with successful applications of these models in industrial settings. The industrial applications include Oil & Gas upstream operations, material blending facilities, natural gas plant design, biofuels synthesis, supply chain facility network design, water network design, industrial electricity market integration, reliable plant design, and supply chain design. Strategies for improving model tractability have been presented, including model linearization, decomposition methods, scenario subset selection, and strengthening cuts, among others. Continuous and discrete optimization in industrial applications remains a rich and thriving field of research with new problems being engaged every year. Algorithmic improvements over the years have made it possible to solve larger models. Some key challenges that are being and need to be tackled are: 1) finding improved relaxations for global optimization, 2) improving the computational performance of large-scale nonconvex MINLP/GDP and stochastic programming, 3) developing algorithms for mixed-integer dynamic optimization that enable integration amongst the three levels of the decision-making pyramid, 4) optimizing entire supply chains, and 5) extending the work to include sustainable system design and operation. Further developments in these areas will greatly improve the quality of decisions that need to be made in the processing industries.

6. Acknowledgements

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