Optimizing chemical processes

Although the methods originated in mathematics and operations research, chemists and engineers are finding these techniques invaluable for process design and synthesis, planning and scheduling, and process control and operation.

Ignacio E. Grossmann
Lorenz T. Biegler

Increased pressure to reduce costs, improve product quality, and minimize environmental risks provided the motivation for development of optimization tools to identify better solutions for the complex problems of plant operation and design. Several factors have contributed to these developments. First, the wide availability of computers and their impressive growth in computational power have promoted the application of mathematical models. Second, improved models have been developed for predicting the performance and economics of chemical processes as well as for embedding many alternatives. Third, recently developed software for optimization has provided new tools for using these models to identify improved solutions. In fact, many of the current decisions in industry regarding process design and operation are being determined through optimization models and techniques, which have relied on a combination of new developments in optimization algorithms, modeling systems, and computer architecture and software.

Although most mathematical techniques were developed by researchers in operations research, numerical analysis, and computer science, chemical engineers played a prominent role in some of these developments (in fact, a significant percentage of operations researchers are chemical engineers). Here we provide a general survey of optimization in chemical engineering, emphasizing the most significant developments over the past 10 years. We review some classes of models and techniques and the research work being conducted in this growing field. We also highlight applications in the areas of process design and synthesis, planning and scheduling, and process control and operation. Finally, we discuss emerging research trends in optimization.

What type of problem is it?

If one assumes no special structure for the problem stated in the model (see box) or to its various particular cases (e.g., only discrete or only continuous variables), then direct-search techniques are often the easiest methods to apply. They are also the most time consuming. Either systematic or random selection of trial points is chosen to evaluate and improve the objective function. Constraints can also be satisfied, but often with some difficulty (e.g., using penalty functions in which a weighted violation of constraints is added to the original objective function). Perhaps the most popular direct-search method that has emerged recently in chemical engineering is simulated annealing. This method is based on analogies with free energy minimization in statistical mechanics. In principle, the method is easy to apply to problems with simple constraints and will probably find solutions that are close to the global optimum. However, aside from the fact that it often requires many thousands of function evaluations before the likely optimum is found, its performance tends to be highly dependent on the selection of parameters of the algorithm.

The most prevalent approach that has been taken in optimization is to consider particular problem classes of the model depending on the form of the objective function and constraints with which efficient solution methods can be derived to exploit special structures.

The particular case of the model (i.e., best-known case) is the linear programming (LP) problem. The objective function and all the constraints are linear, and all the variables are continuous. The optimal solution to LP problems lies at a vertex of the feasible space. Also, any local solution corresponds to the global optimum. These problems have been successfully solved for many years with computer codes based on the simplex algorithm rooted in linear algebraic methods.

A major change in solution methods is the development of interior point algorithms that rely on nonlinear transformations and whose computational requirements are theoretically bounded by a polynomial expressed in terms of the problem size. Interestingly, this property is not shared by the simplex algorithm, which theoretically may require

The authors are with Carnegie Mellon University.

Concepts in optimization

Bilinear function Function given by the sum of products of two variables.

Constraints Equations and/or inequalities that limit the values of the variables in a model.

Convex function Function that coincides or underestimates all linear interpolations between any two arbitrary points; all linear functions are convex.

Convex region Region in which any linear intepolation obtained from two arbitrary points yields a new point belonging to that region.

Global optimum The solution to the mathematical model such that any other feasible variable values produce a worsening in the objective function value.

Kuhn–Tucker conditions Generalization of the zero-derivative optimality condition to problems with constraints.

Local optimum Solutions such that small perturbations around that point lead to a worsening of the objective function value.

Linear programming (LP) Optimization methods with linear objective function and constraints involving only continuous variables.

Mixed-integer linear programming (MILP) Extension of linear programming that allows some of the variables to take on discrete values (mostly binary).

Mixed-integer nonlinear programming (MINLP) Extension of nonlinear programming that allows some of the variables to take on discrete values (mostly binary).

Nonlinear programming (NLP) Optimization problems with nonlinear objective function and constraints involving only continuous variables.

NP completeness Theoretical characterization of worst case for computational requirements that increase exponentially with problem size.

Optimal control Optimization problems that involve differential and algebraic equations as constraints.

Stochastic optimization Optimization problems in which some of the input data are random or subject to fluctuations.

Traveling salesman Special linear optimization problem that consists of finding the cheapest closed tour in a graph where all nodes must be visited exactly once.

exponential time. Because that performance is rarely observed in practice, further significant advances in solving large-scale problems have been made: The simplex algorithm allows problems with up to 15,000–20,000 constraints to be solved quite efficiently. Interior point methods tend to perform better in problems with up to 50,000–100,000 constraints. The mathematical structure of very specialized cases of LP problems (e.g., network flows in assignment or transportation problems) has been greatly exploited, allowing the development of codes that can be applied to problems involving millions of variables.

A mixed-integer linear program (MILP) is the extension of the LP model that involves discrete variables. This model greatly expands the ability to formulate and solve real-world problems, because logical decisions (those with variables 0 or 1) can be included and discrete amounts can be accounted for. The most common method for solving MILP problems is the branch-and-bound search, which consists of solving a subset of LP subproblems while searching within a decision tree of the discrete variables. The other common approach involves the use of cutting planes that attempt to make the MILP solvable as an LP with the addition of special constraints. Because of the combinatorial nature introduced by the discrete variables in MILP problems, these problems have been very hard to solve. Theoretically, one can show that this class of problems is NP complete; that is, there is no known algorithm whose computational requirements do not exceed a polynomial increase in terms of problem size. Nevertheless, recent advances based on combining branch-and-bound methods with cutting planes, and which have been coupled with advances in LP technology, are providing rigorous optimal solutions to problems that were considered unsolvable 10 years ago.

For a case in which all or at least some of the functions are nonlinear and only continuous variables are involved, the model problem gives rise to nonlinear programming (NLP) problems. For a case in which the objective and constraint functions are differentiable, local optima can be defined by the Kuhn–Tucker conditions, a generalization of the zero-derivative optimality conditions. These are probably the most common types of models in chemical engineering.

Whereas problems involving 100 variables for NLP were considered large 10 years ago, solving problems with several thousand variables is quite common nowadays. Reduced gradient and successive quadratic programming (SQP) techniques, which can be derived by applying Newton's method to the Kuhn–Tucker conditions, emerged as the major algorithms for NLP. Reduced gradient is better suited for problems with mostly linear constraints; SQP is the method of choice for highly nonlinear problems.

One limitation of these methods is that they are only guaranteed to converge to a local optimum. For problems that involve a convex objective function and a convex feasible region, this limitation does not exist, because they exhibit only one local optimum (the global optimum). In practice, proving convexity in a nonlinear problem often is not possible, and therefore finding any local optimum is often considered a satisfactory solution, especially if it yields a significant improvement in the solution. On the other hand, there are applications in which finding the global optimum to nonconvex problems is a major issue. Over the past few years significant progress has been made in developing rigorous methods for globally optimizing problems with special structures (e.g., bilinear functions). Also, stochastic methods such as simulated annealing have been successfully applied to problems involving functions that are inexpensive to evaluate.

The extension of NLP for handling discrete variables yields a mixed-integer nonlinear programming (MINLP) problem, which, in its general form, is identical to the model. MINLP problems were considered unsolvable 10 years ago. New algorithms such as the outer-approximation method and extensions of the Generalized Benders decomposition method emerged as the major methods to solve these problems. These methods, which assume the functions can be differentiated, consist of solving an alternating sequence of NLP subproblems and MILP master problems. The former optimize the continuous variables, and the latter optimize the discrete variables. As in the NLP case, global optimum solutions can be guaranteed

The mathematical model

Optimization problems can generally be formulated with mathematical models that involve continuous and discrete variables. These variables must be selected to satisfy equations and inequality constraints while optimizing a given objective function as expressed by the model below:

$$\begin{aligned} &\min f(x,y) \\ \text{subject to} \quad & h(x,y) = 0 \\ & g(x,y) \le 0 \\ & x \in X,\ y \in Y \end{aligned}$$

The continuous variables are represented by x and the discrete variables by y, both with arbitrary dimensionality. The feasible region for the variables x and y is defined by the following constraints: $h(x,y) = 0$, which describes the performance of a system (e.g., mass, energy balances, design equations); $g(x,y) \le 0$, inequalities that are related to specifications (e.g., minimum purity, maximum throughput). In addition, the variables can be further confined to sets X (typically lower and upper bounds) and Y (specific integers). The former specifies the ranges of values for the continuous variables (e.g., positive flows, minimum/maximum pressures for a chemical reactor), and the latter specifies the discrete choices (e.g., only 0–1 choices for, say, selection or not of a unit or an integer number for number of plates). The model in practice can also be posed as a maximization problem or with inequalities that must be greater than or equal to zero. The form here is used for presentation purposes. Any problem can be converted into that form because maximizing a function is equivalent to minimizing its negative value. Inequalities greater than or equal to zero can also easily be converted to less than or equal to zero.

This mathematical model is technically known as a "mathematical program," and an extensive body of literature exists on this subject. (Reference 1 is a good introduction to models; Reference 2 provides a general review of methods.) From a practical standpoint, the important feature of the model is that it provides a powerful framework for modeling many optimization problems, including design, scheduling, and control. Depending on the application at hand and the level of detail in the equations, the objective function and constraints can be given in explicit or implicit form. Explicit equations are given by mathematical expressions that are often used for simplified models. The time to perform an evaluation of this type of model may be very fast even though it may involve thousands of variables and constraints. Implicit equations arise when detailed and complex calculations must be performed as procedures—in process simulators or differential equation models, for instance. In this case, the dimensionality for the optimization can be greatly reduced, although the time for performing an evaluation of one trial point may require a significant length of time.

Formulating a given decision problem as a mathematical program requires three major assumptions: (a) The criterion for optimal selection can be expressed through one single objective function, (b) the constraints must be exactly satisfied, and (c) the parameters (input data) are deterministic in nature. Of course these assumptions represent oversimplifications of real-world problems. However, extensions based on the model can address some of these issues. For instance, it is possible to relax the assumptions in (a) and (b) through multiobjective optimization methods, whereas the assumption in (c) can be relaxed through stochastic optimization methods.

only for convex problems. Solving problems with 100 to 200 0–1 variables and 1000 continuous variables and constraints have been reported with these methods. Major difficulties encountered in MINLP include those encountered in MILP (combinatorial nature requiring large computations) and NLP (nonconvexities yielding local solutions).

Finally, all the aforementioned methods assume that the problem is expressed through algebraic equations. Very often, however, these models involve differential equations as constraints, giving rise to problems known as optimal control problems or the optimization of differential algebraic systems. Major approaches to solving these is to approximate the differential equations by algebraic equations, which then yields solvable NLP problems, or to solve the differential model in a routine that is then treated by the optimizer as a procedure (or implicit function).

Increased computational power and the advent of powerful modeling systems have accelerated advances in optimization techniques. The modeling systems have made an enormous impact in practice with software systems to formulate optimization problems easily in equation form, readily accessible to many users of PCs, workstations, and mainframes. By separating the declarative part of a problem from the solution algorithms and their computer codes, these nonprocedural modeling systems allow users to concentrate on the formulation of models. These systems have reduced the time required by users to formulate optimization problems by at least one order of magnitude. For instance, in the past, the equations of a model and analytical derivatives had to be supplied through subroutines or clumsy data files. This process was not only time consuming but also prone to many errors. Current modeling systems have virtually eliminated many of these problems and greatly facilitate the formulation and solution of optimization problems. Some of the commercial optimization packages for solving the various types of models discussed in this section, as well as equation-based modeling packages and process simulators with optimization capabilities, are shown in the box.

Process design

For three decades, chemical engineers have relied on process simulators to predict the steady-state performance of dedicated large-scale continuous processes (e.g., commodity and petrochemical processes). Traditionally these simulators ran different case studies to select economically attractive alternatives for design. The drawback of such an approach is that the user has to identify the different process configurations and design parameters for the cases to be simulated. Because of time limitations, relatively few cases are examined, which means that some potentially improved designs are commonly overlooked. Furthermore, design problems frequently require satisfying specifications on output streams (e.g., product purity), usually requiring many iterative computations.

For the case of fixed-process configurations, the limitations of the traditional methods have been overcome with the incorporation of efficient NLP optimization strategies using the SQP algorithm. The major challenge overcome here was how to interface the "black box" simulator with the mathematical optimization algorithm that requires derivatives. These developments with NLP optimization allowed the automated manipulation of design parameters

Commercial optimization software

Linear and mixed-integer linear programming (LP, MILP) CPLEX, LAMPS, LINDO, MPSIII, OSL, SCICONIC, XA, XPRESS, ZOOM

Nonlinear programming (NLP) CONOPT, DMO, GRG2, LANCELOT, MINOS, NOVA, NPSOL, RND/OPT, SRQP

Mixed-integer nonlinear programming (MINLP) DICOPT

Modeling systems AMPL, DMO, NOVA, GAMS, SPEED-UP, XPRESS-MP

Process simulators with optimization capability ASPEN, PRO/II, ProSim, HySim

and satisfaction of constraints for optimizing process flow sheets with simulators. Today most commercial simulators have implemented an NLP optimization capability. Computational requirements are only 10–20 times larger than the time required for a single simulation. The process of producing ammonia is one example (Figure 1) (*3*). The parameters of the model were set as:

	Max(before-tax profit at 15% over 5 years)
subject to	NH_3 in purge < 4.5 mol/h
	No liquid in compressors
	100,000 tons NH_3 product purity >99.9%
	$1.8 < H_2/N_2$ in <3.5 combined feed

The results, which were obtained on a process simulator with the SQP algorithm for NLP, are given in Table 1.

Another development in this area was the move from traditional sequential modular simulators toward equation-oriented systems. This change introduced considerable flexibility in process modeling because the specifications can be varied. On the other hand, as opposed to the case of modular simulators, in which the dimensionality of the NLP problem is kept relatively small (few tens of equations and variables), the NLP model in full equation form resembles the form of the model shown earlier. Thus, it commonly involves several hundreds or thousands of equations and variables. The advantage, however, is that analytical derivatives are readily available in these systems. The equation-oriented modeling framework has been particularly successful in optimizing operating conditions of distillation columns and steam and power systems.

Process synthesis

In addition to the optimization of fixed flow sheets, the systematic selection of process configurations (commonly known as process synthesis) has been the subject of considerable research work over the past two decades. Many different approaches have been explored that rely on heuristics, physical insights, and optimization. The optimization models aim at explicitly modeling discrete decisions with 0–1 variables (exclude or include a unit) and continuous variables for the state and design variables, which conceptually gives rise to an MINLP problem, as described earlier.

Significant progress has been made in the area of synthesis of heat recovery networks, for which some powerful insights have been developed through the concept of the pinch point, which defines the bottleneck for maximum heat integration that can be achieved in practics. These heat integration techniques have been extensively applied in industry. The role of optimization in this area has been to automate and expand the scope of these techniques. LP and MILP techniques have been used for targeting energy levels and predicting required stream matches accounting for constraints; MINLP techniques have been used to synthesize network configurations automatically. Figure 2 (p. 32) presents an example of a network involving five hot and five cold streams that was automatically synthesized with the MINLP code DICOPT++ on an IBM RS-6000 (*4*). The model consisted of 135 binary variables, 635 continuous variables, and 850 constraints. The network configuration was selected from a superstructure of alternatives by minimizing the cost of the exchangers and the cost of the steam and cooling water. Optimization techniques are also being applied to the synthesis of reactor and separation systems, although they tend to be considerably more difficult to model as a result

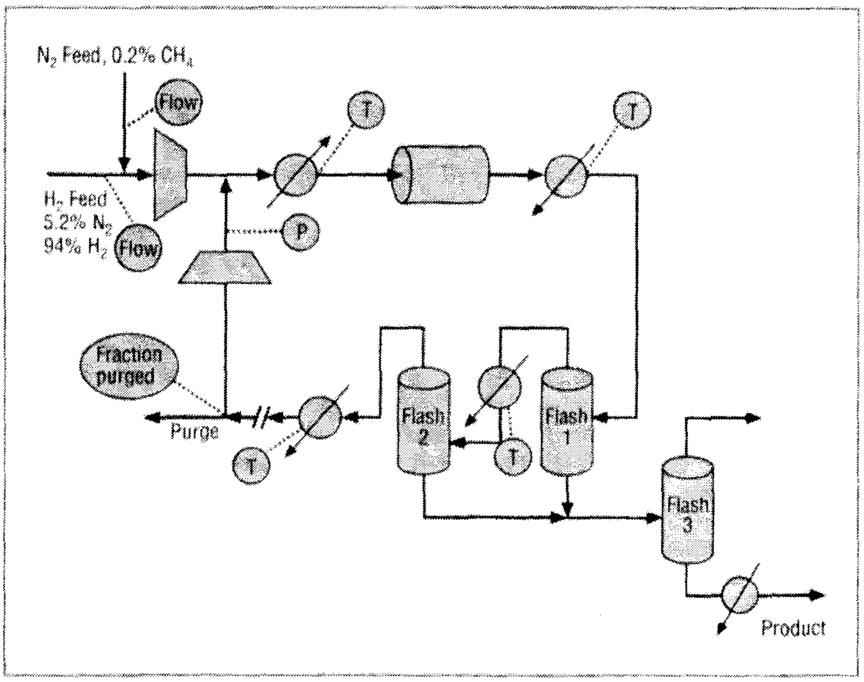

***Figure 1.* Ammonia process flow sheet.** The results of the optimization of this process are shown in Table 2. T, temperature; P, pressure.

Optimization algorithms

Branch and bound Algorithm for MILP that involves enumeration and bounding of a tree search to find the optimum integer solution.

Cutting planes Additional constraints that are added to MILP problems to improve their LP approximation when all variables are treated as continuous variables.

Generalized Benders decomposition Algorithm for NLP, MILP, and MINLP that involves decomposition in which variables are partitioned into complicating and noncomplicating variables.

Interior point algorithm Algorithm for LP that performs Newton iterations on the Kuhn–Tucker conditions avoiding vertex searches.

Outer approximation Algorithm for MINLP that involves accumulation of linearizations to bound the objective function and feasible region.

Reduced gradient Algorithm for NLP that performs Newton iterations in the reduced variable space defined by the degrees of freedom.

Simplex algorithm Algorithm for LP that searches vertices or intersections of constraints to find the optimum.

Simulated annealing Algorithm for nonlinear and discrete optimization that involves generating trial points by simulating the cooling or annealing of a substance.

Successive quadratic programming (SQP) Algorithm for NLP that involves successive Newton iterations of the Kuhn–Tucker conditions.

of the complexity of the equations. Also, several prototypes based on MINLP techniques have been developed for synthesizing configurations of process flow sheets.

Although optimization-based tools for process synthesis are still largely in the research phase, some of them are being transferred to process simulators. One good example is the simultaneous optimization and heat integration of flow sheets. Raw materials are saved significantly through increased recycles and efficient heat recovery.

MINLP techniques have been applied to the discrete design optimization of distillation columns. MINLP optimization models for both feed tray location and number of trays for single and multiple feeds were developed recently within equation-oriented systems using tray-by-tray models with nonideal thermodynamics. Figure 3 (p. 32) shows the optimization of the number of trays as well as the feed tray location in a distillation column with three different feeds for separating methanol and water (*5*). The column shown in this figure considers a maximum of 60 trays with the option of putting the feed in at each tray. The return of the reflux is also considered in principle at each tray to optimize the actual number of trays used. In this case, the optimal number is 53, and the feed trays are located at trays 4, 6, and 12. The full MINLP model, which incorporates the virial and UNIQUAC equations for predicting the thermodynamic properties, has embedded 400,000 alternative designs for the 115 binary variables, 1683 continuous variables, and 1919 constraints. The algorithm in the program DICOPT++ (run on an HP 9000/730), however, required the detailed analysis of only seven designs to find the optimum.

Finally, two important capabilities have started to emerge from academic research: methods for global optimization and methods for design under uncertainty. In the former, the initial trend was to rely on statistical techniques such as simulated annealing. Although these techniques have the advantage of not assuming special forms for the functions, they can be very expensive computationally because they often require many thousands of function evaluations. Therefore, another trend that has emerged is to develop global optimization methods that exploit specific structures, such as the presence of bilinear equations, which are quite prevalent in many process models. Significant progress is being made in this area.

The above examples deal with systems in which input data and models are deterministic. For handling uncertainty in design, deterministic quantitative measures for flexibility have emerged that involve the solution of LP, NLP, and mixed-integer problems. These flexibility measures can be incorporated within design models to ensure feasibility of operation over a specified parameter range. The other approach has been to rely on stochastic optimization methods by treating the uncertain parameters as

***Table 1.* Results of ammonia flow sheet optimization problem**

Item	Optimum	Starting point	Lower bound	Upper bound
Objective function, $10^6/year	26.9286	20.659		
Design variables				
Inlet temp of reactor, °F	400	400	400	600
Inlet temp of first flash, °F	65	65	65	100
Inlet temp of second flash, °F	35	35	35	60
Inlet temp of recycle compressor, °F	80.52	107	60	400
Purge fraction, %	0.0085	0.01	0.005	0.1
Inlet pressure of reactor, psia	2163.5	2000	1500	4000
Flow rate of feed 1, lb·mol/h	2629.7	2632.0	2461.4	3000
Flow rate of feed 2, lb·mol/h	691.78	691.4	643	1000

Source: Reference 3.

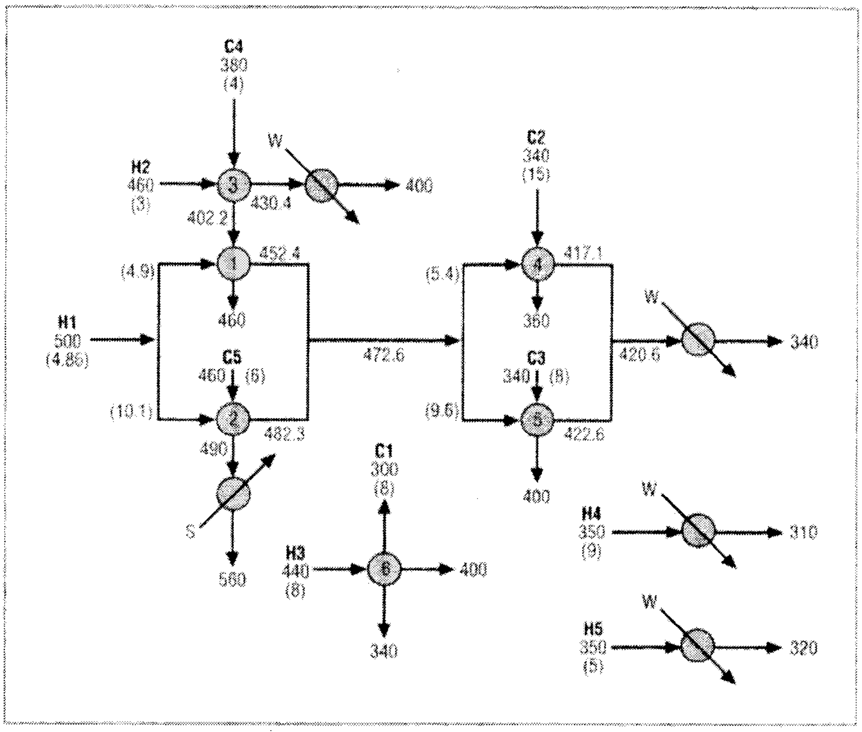

Figure 2. **Automated synthesis of a heat exchanger network involving five hot and five cold streams.** Temperatures of the various streams are shown. Network parameters: total heat exchanger area = 106.7 m^2; heater heat load = 420 kW; cooler heat load = 1810 kW; utilities costs = \$70,600/year; capital investment costs = \$32,027/year. Numbers in parentheses indicate flow (in kW/K). W, water; S, steam.

random variables. The computational expense, however, is still rather high with these techniques.

Planning and scheduling

In the past, optimization techniques and models were applied extensively to production planning and scheduling, in which important plantwide problems such as delivering raw materials, managing inventories, and satisfying product demands are addressed. The models for this application are often linear and quite large and usually were solved using LP methods. The management of the model information is frequently the most time-consuming task. Planning problems are frequently solved for horizons of several weeks to a year with scheduling subproblems for time scales of a week or so.

New NLP optimization models that can capture more precisely the nonlinearities inherent in chemical processes are gradually replacing these LP models. Not that LP models are no longer used: Their use has expanded for strategic long-range planning applications for new investment decisions and for corporate-wide production planning and distribution. Furthermore, the usefulness of these models has been augmented by the increasing power of MILP techniques with which discrete decisions and discontinuous functions can be modeled.

A growth area that has emerged for optimization over the past few years is the scheduling of batch processes. Traditionally these problems were addressed with heuristcs and intuition because they represent a class of problems with a large number of possible combinations. However, pressures for improving product deliveries and reducing inventories and costs increased the need for systematic optimization techniques for scheduling. In addition, increased complexity in the flexible operation of batch manufacturing facilities made development of these techniques a priority.

Optimization models for batch scheduling tend to be linear, highly structured, and very large. For example, finding the best sequence of batches in a sequential multi-

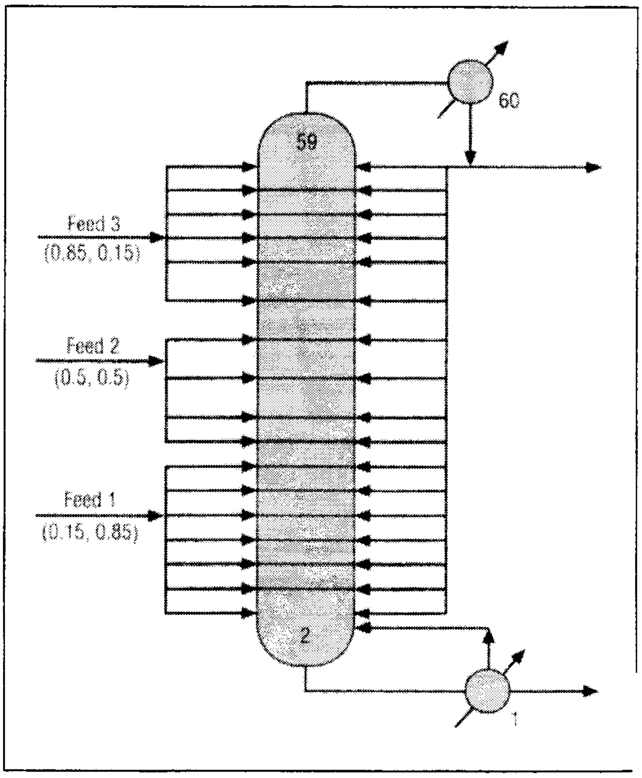

Figure 3. **The optimal number of plates and feed locations in a distillation column with multiple feeds can be determined.** For this example, a separation of methanol–water with three feeds was optimized. Numbers in parentheses indicate percentages of methanol and water, respectively.

product plant gives rise to an asymmetric traveling salesman problem. If you are dealing with the scheduling of 20 batches, 400 logical (0–1) variables are required; if you are dealing with 100 batches, 10,000 variables are needed. Successful implementation of a parallel branch-and-bound method has been developed for solving these problems

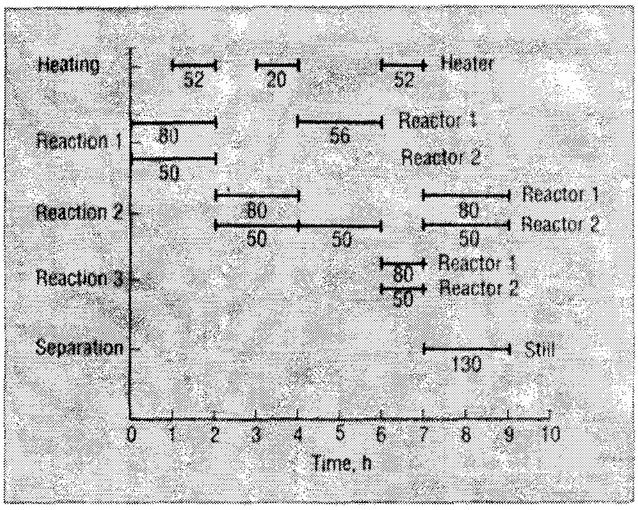

Figure 4. **Gantt chart for the optimal scheduling of a batch plant.** Tasks are indicated at left and equipment at right. Numbers under lines indicate quantities being processed.

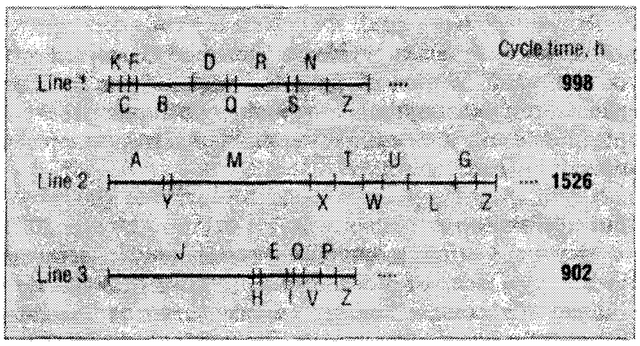

Figure 5. **Cyclic scheduling of polymer production in parallel lines.** Each letter indicates a particular product.

and applied in industry. These models have handled as many as 49,000,000 binary variables. Again, an alternative technique for solving these problems is simulated annealing. In addition to the highly structured optimization problems, MILP techniques are being used to handle more general cases. Especially noteworthy is the state–task–network model, which allows the modeling of more complex plant configurations and operations as well as the handling of resource constraints. A Gantt chart of a schedule that was obtained with this approach is shown in Figure 4 (*6*).

Scheduling problems are usually easy to state but at the same time very diverse. Thus, it is difficult to develop single unified model representations. For example, the methodologies described in the previous paragraph apply to day-to-day operations with short-term scheduling in which detailed decisions are required at each point in time within the specified time frame. For long-term strategic studies, the trend is to develop models that involve cyclical schedules and integrate production planning considerations to decide how much to produce in the first place. These optimization problems often give rise to MILP and MINLP models. Successful solution through decomposition techniques has been reported for the case of continuous multiproduct plants with parallel production lines. Sahinidis and Grossman (*7*) reported application to a real-world problem with an MINLP model involving as many as 800 binary variables and 23,000 continuous variables. That model was solved as shown in Figure 5, in which the optimal assignment and sequence of 26 polymer products, as well as the length of cycle times, were determined for a plant consisting of three parallel lines.

Process control and operation

Computer-based, integrated systems in process operations and control have supplanted classical control approaches and hardware. As a result, general and powerful algorithms now can be applied without hardware limitations. Thus, many process companies have developed a hierarchy of tasks for process operations that applies optimization tools at multiple levels leading to a general, systematic strategy for improved operation and control. These levels include the overall logistics for process planning and scheduling as well as steady-state optimization for plant operation and process control.

After planning and scheduling decisions are made over a longer time frame, the day-to-day task of determining an operating policy is required. For the batch processes discussed earlier, operations are determined by a fixed, often inflexible, recipe. In continuous processes, there is much more flexibility for operation and adjustment; therefore, detailed, nonlinear steady-state process models are constructed, and a quantitative objective (e.g., minimize utilities, maximize production, maximize profit) can be optimized. Although on-line operations modeling and optimization have been applied in some companies for over a decade, it is relatively new and has found widespread use only in the past five years.

Because the purpose of process operations modeling is different from process design, less-detailed models are frequently used, and there is still a tendency to "tailor make" these models for each plant. Moreover, unlike process design models, operations models often are represented in equation-based or "open" form. This open-form approach has been extended even to reactor models described by differential equations; these equations have been discretized to algebraic equations, resulting in increased problem size. Characteristics of these operating models include sparse linear and nonlinear equations that consist of tens of thousands of equations and variables and relatively few degrees of freedom (typically <100), which include process adjustments in flow rates, temperatures, and pressures. Moreover, in contrast to design calculations, there is less reliance on detailed physical property models (e.g., for vapor–liquid equilibrium) and more emphasis on tuning parameters that update the model with changes in process conditions. Large-scale adaptations of the SQP algorithm have been used to solve these models in most applications, but successful applications of reduced gradient algorithms have also been reported. The small real-time optimization problem shown in Figure 6 (p. 34) has about 3000 variables and equations (*8*). It is up to two orders of magnitude smaller than many plantwide applications, but it shares many characteristics and functional forms with these applications.

The straightforward application of NLP strategies has led to significant performance improvements in many processes, without additional capital expenditures and very short payout times. In Table 2 (p. 35) we list several applications of real-time optimization reported in the recent literature (*9*). The problem size, location, company where it was applied, and reported operating benefits are reported when available.

A suitable objective for process control is the minimization of the output deviation from a desired setpoint over a

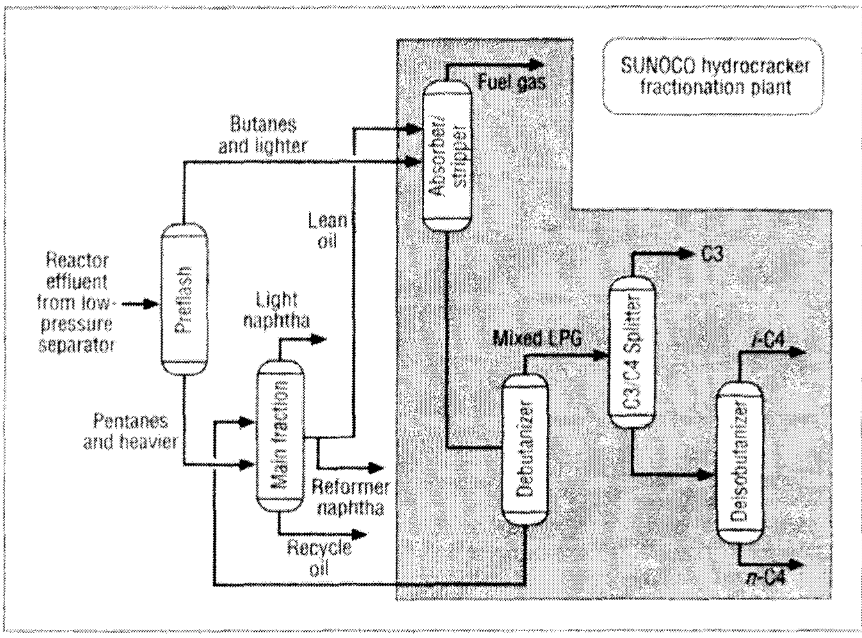

Figure 6. **SUNOCO hydrocracker fractionation plant, a relatively small real-time optimization problem with about 3000 variables and equations.**

predicted time frame, and this function is often stabilized with a quadratic penalty of the input moves. Furthermore, constraints on inputs and outputs that arise from process considerations can be easily added to the problem formulation. Such a formulation yields a linear or quadratic programming problem, and efficient finite-step algorithms are often used to solve these problems on-line. In this way, a general optimization-based strategy can be applied to a variety of different process units, and the problem of controller design is greatly simplified. This approach is referred to as model predictive control (MPC), and a number of variations have been derived in industry and academia.

Accurate representations

Both the steady-state optimization and model predictive control tasks are crucially dependent on an accurate model representation of the plant. These tasks of parameter and state estimation involve questions of the efficiency of computation (based on problem structure), statistical inference of the model parameters, the detection of data outliers, and robust and stable implementation and behavior of these algorithms.

In experimental chemistry, parameter estimation is an essential tool in determining underlying reaction rate constants as well as transport and thermodynamic parameters from data obtained in well-planned experiments. Moreover, this task is necessary in the elucidation of fundamental models and discrimination among competing models. Finally, parameter and state estimation is essential to provide a predictive capability to any fundamental or empirical model. Applications of these approaches range from determining the performance of a small bench-scale reactor to the large-scale partial differential equation models used in weather forecasting. Linear parameter estimation problems are solved directly by linear least squares algorithms. Nonlinear (and constrained) parameter estimation problems are frequently solved using the same NLP tools used for the on-line optimization; these are solved with SQP. More efficient SQP strategies tailored to parameter estimation can also be applied by taking advantage of the "least squares" structure of these problems. In this way, parameter estimation problems can often be solved with only a small fraction of the effort required for the more general nonlinear optimization problems. Similar issues on parameter and state estimation problems arise in process operations and control.

Future research

The scope of these optimization techniques is increasing greatly as a result of a combination of theoretical and algorithmic advances, which are complemented by the rapid progress in computer hardware and software. Optimization is a very active area of research in academia and in industry. Here are some of the major trends that we foresee in the area of optimization and ideas about how they will help the designer of chemical products and processes.

Large-scale models. As the power of computer hardware and optimization algorithms increases, there is an increasing demand for solving larger and more complex problems. During the past 15 years the solvable optimization problem has increased in size by two to three orders of magnitude. It is expected that this trend will continue (and even perhaps accelerate) during the next few years and that advanced computer architectures (e.g., parallel computing) will play a major role. In addition, in a number of applications, the bottleneck is no longer the solution of large problems but the handling of massive amounts of data needed to formulate these problems.

Model-building tools. As the capability of solving large-scale problems becomes more widely available, the need for powerful and easy-to-use modeling tools becomes more important. This is currently an active area. Systems are being developed that can automatically generate large algebraic models from high-level representations, perform differentiation, and run on multiple platforms ranging from PCs to supercomputers.

Global optimization. Nonlinear optimization techniques have long relied on finding local solutions. This capability will continue to be important in a number of applications. However, there is also an increasing trend to develop global optimization techniques that are both stochastic and deterministic in nature. Because of their large computing requirements, these methods will benefit from

Table 2. **Case studies for real-time optimization**

Company	Application	Results
Amoco	Gas plant	$4.0 million/year
British Petroleum	Refinery	$2.5 million/year
Chevron USA	Ethylene plant	5–10%
Lyondell	Ethylene plant	9-month payout
ÖMV Deutschland	Ethylene plant	1–3%
Star Enterprise	Crude unit	$3.0 million/year
Shell Oil	Ethylene plant	$4.0 million/year
Shell	Oil refinery	9% in gasoline production
Texaco	Refinery	$4.0 million/year
Wilton	Power station	2–6%

Problem characteristics: 8000–20,000 equations; <40 degrees of freedom.
Source: Reference 9.

advances in high-performance computing. Global optimization methods are expected to have a large impact in applications such as molecular design and process synthesis because these problems often have local solutions that are not meaningful.

Design under uncertainty. The treatment of uncertainties in optimization, especially through stochastic methods, has been computationally very time consuming, often too costly to solve. Advances in computing and new algorithms hold promise for anticipating the effect of uncertainties in optimization problems for design, planning, and operation. This area will also be driven by needs to increase quality in chemical processes.

Product design. Aside from applications in process control and process operations, most of the work in the area of optimization has concentrated on process design. Very little has been done to apply optimization to the design of products. One of the trends beginning to emerge is the application of optimization techniques to molecular design problems.

Integration of models. There will probably be major developments in the area of integration of planning, scheduling, and control in operational problems. In the design area, a major challenge that remains is the integration of process synthesis with process simulation, in which complex models are used at the stage of selecting process alternatives. Another area is the integration of operational considerations, such as scheduling and control, at the design stage.

Integration of methods. Synergy and integration of methodologies are required to increase the scope and power of problem-solving techniques. One trend is to combine quantitative based mixed-integer programming techniques with symbolic techniques based on propositional logic. Another trend is toward "cooperative problem-solving schemes," in which various methods are applied simultaneously to the solution of a given problem.

An exciting future

We hope to have conveyed both the excitement of this growing field and an understanding and appreciation for some of its research and development issues. The computer programs that are an integral part of the chemical processing industry today are growing increasingly more powerful, and their growth is a result of the research and mathematical methods we presented. The examples given here have shown that significant progress has been made, especially in view of the fact that many of the methods were nonexistent 15 years ago. Clearly, optimization is a useful and practical methodology in the chemical industry with a long and promising future ahead.

References

(1) Williams, H. P. *Model Building in Mathematical Programming*; Wiley-Interscience: New York, 1985.
(2) Nemhauser, G. L.; Rinooy Kan, A.H.G.; Todd, M. J. *Optimization*; North Holland: Amsterdam, The Netherlands, 1989.
(3) Lang, Y. D.; Biegler, L. T. *Comp. Chem. Eng.* **1987**, *11*, 143.
(4) Bolio, B.; Yee, T. F.; Grossmann, I. E. *SYNHEAT Manual*; Carnegie Mellon University: Pittsburgh, PA, 1992.
(5) Viswanathan, J.; Grossmann, I. E. *Comp. Chem. Eng.* **1993**, *17*, 949.
(6) Kondili, E.; Pantelides, C. C.; Sargent, R.W.H. *Comp. Chem. Eng.* **1993**, *17*, 211.
(7) Sahinidis, N. V.; Grossmann, I. E. *Comp. Chem. Eng.* **1989**, *13*, 1049.
(8) Bailey, J. K.; Hrymak, A. N.; Treiber, S. S.; Hawkins, R. B. *Comp. Chem. Eng.* **1993**, *17*, 123.
(9) Lauks, U. E.; Vasbinder, R. J.; Valkenburg, P. J.; van Leeuwen, C. *Chem. Eng. Prog.* **1992**, *16*, S213–20.

Ignacio E. Grossmann is the Rudolph R. and Florence Dean Professor of Chemical Engineering and department head at Carnegie Mellon University (Pittsburgh, PA 15213; 412-268-2230). His research is aimed at the development and application of mixed-integer linear and nonlinear programming techniques for process synthesis, batch design, planning, and scheduling. His interests also include energy integration and the design of flexible systems. He has written more than 130 technical publications. He is co-director of the Computer-Aided Process Design Consortium at Carnegie Mellon. He earned his Ph.D. in chemical engineering at Imperial College (U.K.). Send e-mail to <grossmann@cmu.edu>.

Lorenz T. Biegler is professor of chemical engineering at Carnegie Mellon University. His research is aimed at the development and application of nonlinear programming algorithms for flow sheet optimization, parameter estimation, and optimal control. He is also interested in reactor network synthesis and nonlinear process control. He has written more than 100 technical publications. He is the current vice-president of Computer Aids for Chemical Engineering Education (CACHE) and co-director of the Computer-Aided Process Design Consortium at Carnegie Mellon. He obtained his Ph.D. in chemical engineering from the University of Wisconsin. Send e-mail to <biegler@cmu.edu>.