

Chapter 1

Introduction

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1.1 Process Optimization

Optimization refers to finding the values of decision (or free) variables, which correspond to and provide the maximum or minimum of one or more desired objectives. It is ubiquitous in daily life - people use optimization, often without actually realizing, for simple things such as traveling from one place to another and time management, as well as for major decisions such as finding the best combination of study, job and investment. Similarly, optimization finds many applications in engineering, science, business, economics, etc. except that, in these applications, quantitative models and methods are employed unlike qualitative assessment of choices in daily life. Without optimization of design and operations, manufacturing and engineering activities will not be as efficient as they are now. Even then, scope still exists for optimizing the current industrial operations, particularly with the ever changing economic, energy and environmental landscape.

Optimization has many applications in chemical, mineral processing, oil and gas, petroleum, pharmaceuticals and related industries. Not surprisingly, it has attracted the interest and attention from many chemical engineers in both the academia and industry for several decades. Optimization of chemical and related processes requires a mathematical model that describes and predicts the process behavior.

Process modeling and optimization along with control characterizes the area of process systems engineering (PSE), important in chemical engineering with a wide range of applications. The significant role of optimization in chemical engineering and contributions of chemical engineers to the field can be seen from the many books written by chemical engineering academicians (e.g., Lapidus and Luus, 1967; Beveridge and Schechter, 1970; Himmelblau, 1972; Ray and Szekely, 1973; Floudas, 1995 and 1999; Luus, 2000; Edgar *et al.*, 2001; Tawarmalani and Sahinidis, 2002; Diwekar, 2003; Reklaitis *et al.*, 2006). Besides these books devoted entirely to optimization, several books on process design cover optimization too (e.g., Biegler *et al.*, 1997; Peters *et al.*, 2003; Seider *et al.*, 2003).

The main focus of optimization of chemical processes so far has been optimization for one objective at a time (i.e., single objective optimization, SOO). However, practical applications involve several objectives to be considered simultaneously. These objectives can include capital cost/investment, operating cost, profit, payback period, selectivity, quality and/or recovery of the product, conversion, energy required, efficiency, process safety and/or complexity, operation time, robustness, etc. A few of these will be relevant for a particular application; for example, see Chapter 2 for the objectives (typically 2 to 4) used in each of the numerous chemical engineering applications summarized.

The appropriate objectives for a particular application are often conflicting, which means achieving the optimum for one objective requires some compromise on one or more other objectives. Some examples of sets of conflicting objectives are: capital cost and operating cost, selectivity and conversion, quality and conversion, profit and environmental impact, and profit and safety cost. These conflicting objectives can be handled by combining them suitably into one objective. A classic example of this practice is the use of total annual cost which includes operating cost and certain fraction of capital cost. The latter depends on plant life, expected return on investment and maintenance cost. Although the fraction of capital cost to be included in the total annual cost can be estimated, will it not be better to have a range of optimal solutions with varying capital and operating costs? Managers and engineers will then be able to choose one of the optimal solutions with the full knowledge on the variation of conflicting objectives besides

their own experience and other considerations which could not be included in the optimization problem.

Multi-objective optimization (MOO), also known as multi-criteria optimization, particularly outside engineering, refers to finding values of decision variables which correspond to and provide the optimum of *more than one objective*. Unlike in SOO which gives a unique solution (or several multiple optima such as local and global optima in case of non-convex problems), there will be many optimal solutions for a multi-objective problem; the exception is when the objectives are not conflicting in which case only one unique solution is expected. Hence, MOO involves special methods for considering more than one objective and analyzing the results obtained.

The relevance and importance of MOO in chemical engineering is increasing, which has been partly motivated by the availability of new and effective methods for solving multi-objective problems as well as increased computational resources. The study of Bhaskar *et al.* (2000) shows that there were around 30 journal publications on applications of MOO in chemical engineering before year 2000 (i.e., excluding those published in 2000). On the other hand, as will be shown in Chapter 2, nearly 100 MOO applications in chemical engineering have been studied and reported in more than 130 journals from the year 2000 to mid 2007. Another evidence of increasing interest and importance of MOO in chemical engineering is the inclusion of a chapter on MOO in the recent book on optimization by Diwekar (2003). Further, there have been several books on MOO outside the chemical engineering discipline (e.g., Cohon, 1978; Hwang and Masud, 1979; Chankong and Haimes, 1983; Sawaragi *et al.*, 1985; Stadler, 1988; Haimes *et al.*, 1990; Miettinen, 1999; Deb, 2001; Coello Coello *et al.*, 2002; Tan *et al.*, 2005). Understandably, their scope does not specifically include chemical engineering applications. The present book, that you are reading now, is the first book entirely devoted to MOO techniques and applications in chemical engineering.

The rest of this chapter is organized as follows. The next two sections respectively cover basics and methods for MOO. In the fourth section, optimization of a typical process for multiple objectives is described. The scope and organization of this book that includes an outline of individual chapters are presented in the last section.

1.2 Multi-Objective Optimization: Basics

In general, a MOO problem will have two or more objectives involving many decision variables and constraints. For illustration, consider an MOO problem with two objectives: $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$, and several decision variables (\mathbf{x}). Such problems are known as two- or bi-objective optimization problems.

$$\text{Minimize } f_1(\mathbf{x}) \quad (1.1a)$$

$$\text{Minimize } f_2(\mathbf{x}) \quad (1.1b)$$

With respect to \mathbf{x}

$$\text{Subject to } \mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U \quad (1.1c)$$

$$h(\mathbf{x}) = \mathbf{0} \quad (1.1d)$$

$$g(\mathbf{x}) \leq \mathbf{0} \quad (1.1e)$$

Some applications may involve maximization of one or more objectives, which can be re-formulated by multiplying by -1 or taking the reciprocal (while ensuring that the denominator does not become zero) as the objective to be minimized. Hence, the above problem with two objectives to be minimized can be used for discussion without loss of generality.

The decision variables can either be all continuous within the respective lower and upper bounds (\mathbf{x}^L and \mathbf{x}^U) or a mixture of continuous, binary (i.e., 0 or 1) and integer variables. In chemical engineering applications, the equality constraints, $h(\mathbf{x}) = 0$ arise from mass, energy and momentum balances - these can be algebraic and/or differential equations. The inequality constraints, $g(\mathbf{x})$ are due to equipment, material, safety and other considerations. Examples of inequality constraints are the requirement that the temperature in a reactor should be below a specified value to avoid reaction run-away, failure of the material used for equipment fabrication, undesirable side products and so on and so forth. The number of equality and inequality constraints can be none, a few or many depending on the application. The feasible region will be a multi-dimensional space satisfying bounds on variables, equality and inequality constraints. Besides \mathbf{x} , $f(\mathbf{x})$, $h(\mathbf{x})$ and $g(\mathbf{x})$ contain constants and/or parameters whose values are known. Note that MOO can also be used for estimating parameters in models – here, parameters are the decision variables.

The two objectives, $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ are often conflicting. In such situations, there will be many optimal solutions to the MOO problem in equation 1.1. All these solutions are equally good in the sense that each

one of them is better than the rest in at least one objective. This implies that one objective improves while at least another objective becomes worse when one moves from one optimal solution to another. The solutions of an MOO problem are known as the Pareto-optimal solutions or, less commonly, Edgeworth-Pareto optimal solutions after the two economists, Edgeworth and Pareto, who developed the theory of indifference curves in the late 19th century. In the published literature, they are also referred to as non-dominated, non-inferior, efficient or simply Pareto solutions.

Definition: The set: \mathbf{x}^P , $f_1(\mathbf{x}^P)$ and $f_2(\mathbf{x}^P)$ is said to be a *Pareto-optimal solution* for the two-objective problem in equation 1.1, if and only if, no other feasible \mathbf{x} exists such that $f_1(\mathbf{x}) \leq f_1(\mathbf{x}^P)$ and $f_2(\mathbf{x}) \leq f_2(\mathbf{x}^P)$ with strict inequality valid for at least one objective.

Pareto-optimal solutions can be represented in two spaces – objective space (e.g., $f_1(\mathbf{x})$ versus $f_2(\mathbf{x})$) and decision variable space. Definitions, techniques and discussions in MOO mainly focus on the objective space. However, implementation of the selected Pareto-optimal solution will require some consideration of the decision variable values. Multiple solution sets in the decision variable space may give the same or comparable objectives in the objective space; in such cases, the engineer can choose the most desirable solution in the decision variable space. See Tarafder *et al.* (2007) for a study on finding multiple solution sets in MOO of chemical processes.

The Pareto-optimal solutions of an MOO problem (namely, optimization of the classical Williams-Otto process for minimizing payback period, PBP, and maximizing the net present worth, NPW), described in detail in Chapter 10, are shown in Figure 1.1. For the present, in Figure 1.1, only the values of objectives and two decision variables (reactor temperature, T and reactor volume, V) are shown. In this figure, the first plot depicts the objective space and the other plots show the decision variables versus one objective. It is clear that the two objectives are conflicting since PBP increases with NPW. Further, optimal results in Figure 1.1a indicate that PBP increases gradually until $\text{NPW} \approx 7 \times 10^6$ US\$ and then significantly. All of these are of interest to decision makers since both PBP and NPW are the popular economic criteria used for evaluating and selecting projects in industrial setting. As shown in Figures 1.1b and 1.1c, optimal values of decision variables

could vary with the objectives. Thus, the optimal solutions of MOO problems can be represented in two spaces: objective space (Figure 1.1a) and decision variable space (Figures 1.1b and 1.1c). In some publications, optimal values of objectives shown in Figure 1.1(a) are referred to as the Pareto-optimal (or simply Pareto) front. Besides the optimal values of the objectives, optimal values of the decision variables are of interest in selecting and implementing one of the optimal solutions in the industry.

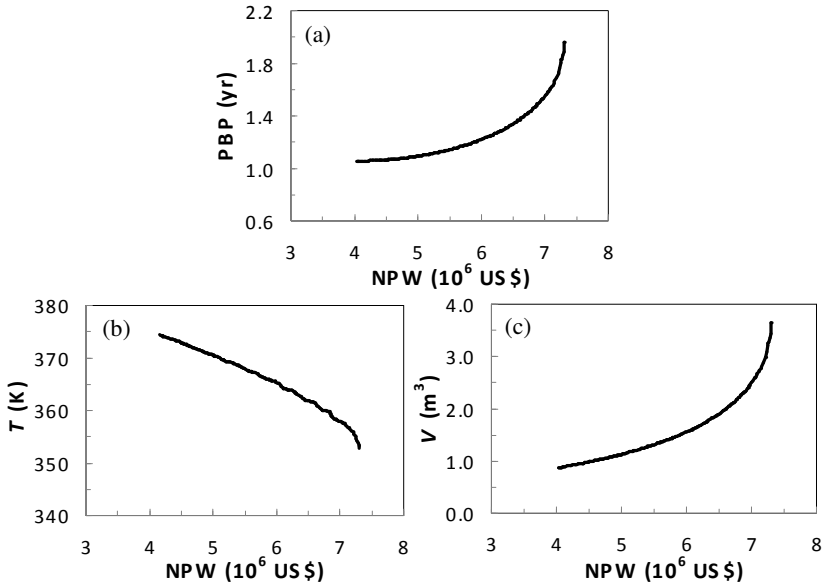


Fig. 1.1 Optimal results of Williams-Otto process for minimizing payback period, PBP and maximizing net present worth, NPW: (a) PBP versus NPW, (b) reactor temperature, T , versus NPW and (c) reactor volume, V , versus NPW.

Pareto-optimal solutions for another example – optimization of the dual independent expander refrigeration system for liquefaction of natural gas for minimizing the total capital cost (C_{total}) and the total shaftwork required (W_{total}), are shown in Figure 1.2. This example is one of the two cases described in Chapter 8. In this case, a kink is observed in the Pareto-optimal front when C_{total} is about 9.7 MM\$ (Figure 1.2a), which corresponds to the point of discontinuity observed in optimal value of one decision variable (Figure 1.2b). The optimal value of another decision variable, on the other hand, is practically constant (Figure 1.2c). Although discrete points are shown in Figure 1.2, the

Pareto-optimal solutions are probably smooth curves except for the discontinuity in Figure 1.2b.

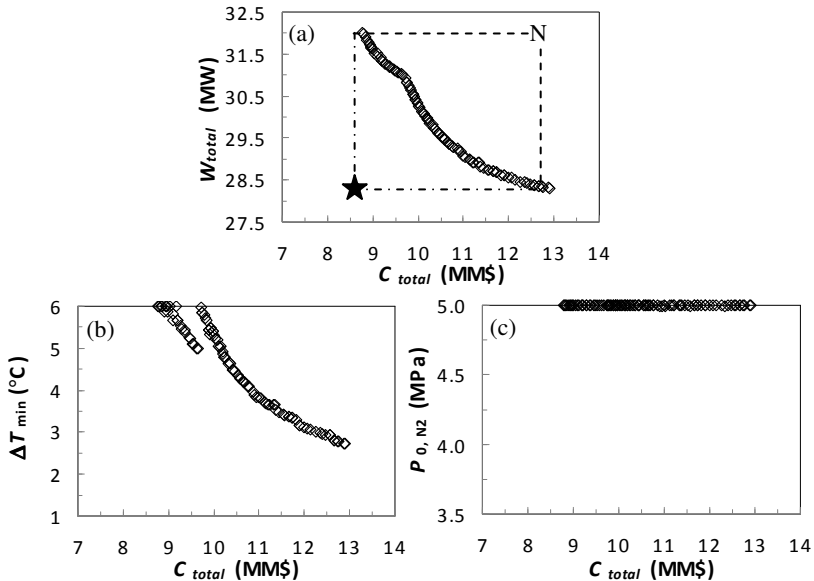


Fig. 1.2 Pareto-optimal solutions for the optimization of the dual independent expander refrigeration process: (a) objectives (W_{total} and C_{total}) to be minimized, and (b) and (c) two decision variables. See Chapter 8 for further details.

In MOO, ideal and nadir objective vectors are occasionally used. The ideal objective vector contains the optimum values of the objectives, when each of them is optimized individually disregarding the other objectives. The ideal objective vector denoted by superscript * (i.e., $[f_1^* f_2^*]$) is shown in Figure 1.2a along with the nadir objective vector denoted by superscript N (i.e., $[f_1^N f_2^N]$). Here, f_1^N is the value of $f_1(\mathbf{x})$ when $f_2(\mathbf{x})$ is optimized individually, and f_2^N is the value of $f_2(\mathbf{x})$ when $f_1(\mathbf{x})$ is optimized individually. Components of the nadir objective vector are the upper bounds (i.e., most pessimistic values) of objectives in the Pareto-optimal set. In case of two objectives, as shown in Figure 1.2a, they correspond to the value of one objective when the other is optimized individually. This may not be the case if there are more than two objectives (Weistroffer, 1985). The ideal objective vector is not realizable unless the objectives are non-conflicting in which case the MOO problem has only a unique solution, namely, ideal objective vector. However, it tells us the best possible value for each of the

objectives. On the other hand, nadir objective vector is not a desirable solution; further, it may or may not be feasible depending on the constraints. Components of both the ideal and nadir objective vectors are useful for normalizing the objectives in some MOO methods.

1.3 Multi-Objective Optimization: Methods

Many methods are available for solving MOO problems, and many of them involve converting the MOO problem into one or a series of SOO problems. Each of these problems involves the optimization of a ‘scalarizing’ function, which is a function of original objectives, by a suitable method for SOO. There are many ways of defining a scalarizing function, and therefore many MOO methods exist. Although the scalarization approach is conceptually simple, the resulting SOO problems may not be easy to solve.

Available methods for MOO can be classified in different ways. One of them is based on whether many Pareto-optimal solutions are generated or not, and the role of the decision maker (DM) in solving the MOO problem. This particular classification, adopted by Miettinen (1999) and Diwekar (2003), is shown in Figure 1.3. The DM can be one or more individuals entrusted with the task of selecting one of the Pareto-optimal solutions for implementation based on their experience and other considerations not included in the MOO problem. As shown in Figure 1.3, MOO methods are firstly divided into two main groups – generating methods and preference-based methods. As the names imply, the former methods generate one or more Pareto-optimal solutions without any inputs from the DM. The solutions obtained are then provided to the DM for selection. On the other hand, preference-based methods utilize the preferences specified by the DM at some stage(s) in solving the MOO problem.

The generating methods are further divided into three sub-groups, namely, no-preference methods, *a posteriori* methods using the scalarization approach and *a posteriori* methods using the multi-objective approach. No-preference methods, as the name indicates, do not require the relative priority of objectives whatsoever. Although a particular method gives only one Pareto-optimal solution, a few Pareto-optimal solutions can be obtained by using different no-preference methods (and so different metrics). Methods in this sub-group include

the method of global criterion and multi-objective proximal bundle method.

The ε -constraint and weighting methods belong to *a posteriori* methods using the scalarization approach. These methods convert an MOO problem into a SOO problem, which can then be solved by a suitable method to find one Pareto-optimal solution. A series of such SOO problems will have to be solved to find the other Pareto-optimal solutions. See Chapter 6 for a discussion of the weighting and ε -constraint methods, their properties and relative merits.

A posteriori methods using the multi-objective approach rank trial solutions based on objective values and finally find many Pareto-optimal solutions. They include population-based methods such as non-dominated sorting genetic algorithm and multi-objective differential evolution as well as multi-objective simulated annealing. In effect, all *a posteriori* methods provide many Pareto-optimal solutions to the DM, who will subsequently review and select one of them for implementation. Thus, the role of DM in these methods is after finding the Pareto-optimal solutions, which justifies their name - *a posteriori* methods. Classifications described in Miettinen (1999) and Diwekar (2003) had only one sub-group for *a posteriori* methods. Here, as shown in Figure 1.3, they are divided into two sub-groups – *a posteriori* methods using the scalarization approach and *a posteriori* methods using the multi-objective approach, for two reasons. Firstly, the methods in the two sub-groups employ different approaches for solving the MOO problems, and, secondly, several methods of this type have been developed and applied to many applications in the past ten years.

Preference-based methods have been divided into two sub-groups: *a priori* methods and interactive methods. In the former methods, preferences of the DM are sought and included in the initial formulation of a suitable SOO problem. Examples of *a priori* methods are value function methods, lexicographic ordering and goal programming. The approach of value function methods involves formulating a value function, which includes original objectives and preferences of the DM for optimization and then solving the resulting SOO problem. Weighting method is one particular case of value function methods. In lexicographic ordering, the DM must arrange the objectives according to their importance for subsequent solution by a SOO method. The DM provides an aspiration level for each of the objectives (whose achievement is the

goal) in goal programming; a suitable SOO problem is then formulated and solved.

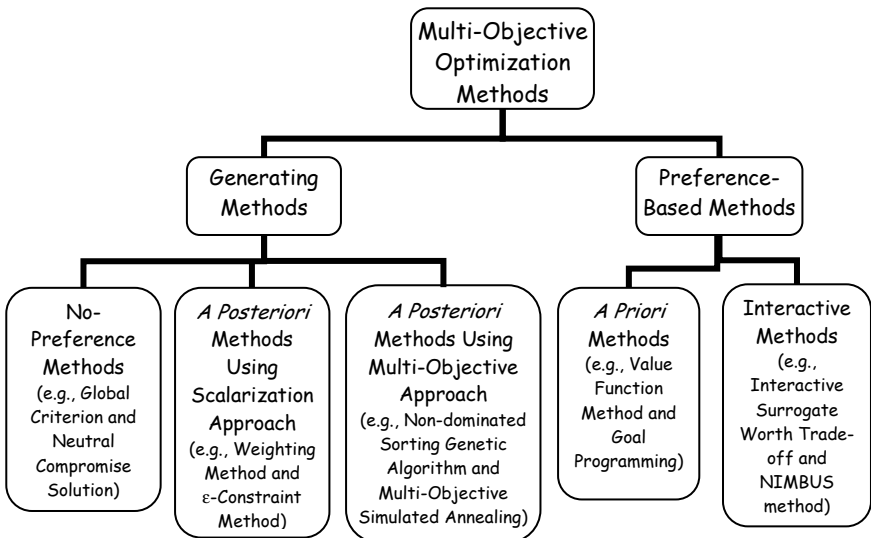


Fig. 1.3 Classification of multi-objective methods.

Interactive methods, as the name implies, requires interaction with the DM during the solution of the MOO problem. After an iteration of these methods, s/he reviews the Pareto-optimal solution(s) obtained and articulates, for example, further change (either improvement, compromise or none) desired in each of the objectives. These preferences of the DM are then incorporated in formulating and solving the optimization problem in the next iteration. At the end of the iterations, the interactive methods provide one or several Pareto-optimal solutions. Examples of these methods are interactive surrogate worth trade-off method and the NIMBUS method, which have been applied to several chemical engineering applications.

The classification in Figure 1.3 takes into account the recent developments and provides a good overview of available MOO methods. Relative merits and limitations of groups of methods are summarized in Table 1.1. A few of the MOO methods can be placed in another group. For example, weighting method in the *a posteriori* methods is a special case of value function methods in the *a priori* methods. The ϵ -constraint method from the *a posteriori* methods and goal programming from

a priori methods have been adopted for developing interactive methods. Thus, classification of MOO methods is somewhat subjective. For details on many methods including their theoretical properties and strengths, interested readers are referred to the comprehensive book by Miettinen (1999).

Table 1.1 Main Features, Merits and Limitations of MOO Methods

Methods	Features, Merits and Limitations
No Preference Methods (e.g., global criterion and neutral compromise solution)	These methods, as the name indicates, do not require any inputs from the decision maker either before, during or after solving the problem. Global criterion method can find a Pareto-optimal solution, close to the ideal objective vector.
<i>A Posteriori</i> Methods Using Scalarization Approach (e.g., weighting and ϵ -constraint methods)	These classical methods require solution of SOO problems many times to find several Pareto-optimal solutions. ϵ -constraint method is simple and effective for problems with a few objectives. Weighting method fails to find Pareto-optimal solutions in the non-convex region although modified weighting methods can do so. It is difficult to select suitable values of weights and ϵ . Solution of the resulting SOO problem may be difficult or non-existent.
<i>A Posteriori</i> Methods Using Multi-Objective Approach (many based on evolutionary algorithms, simulated annealing, ant colony techniques etc.)	These relatively recent methods have found many applications in chemical engineering. They provide many Pareto-optimal solutions and thus more information useful for decision making is available. Role of the DM is after finding optimal solutions, to review and select one of them. Many optimal solutions found will not be used for implementation, and so some may consider it as a waste of computational time.
<i>A Priori</i> Methods (e.g., value function, lexicographic and goal programming methods)	These have been studied and applied for a few decades. Their recent applications in chemical engineering are limited. These methods require preferences in advance from the DM, who may find it difficult to specify preferences with no/limited knowledge on the optimal objective values. They will provide one Pareto-optimal solution consistent with the given preferences, and so may be considered as efficient.
Interactive Methods (e.g., interactive surrogate worth trade-off and NIMBUS methods)	Decision maker plays an active role during the solution by interactive methods, which are promising for problems with many objectives. Since they find one or a few optimal solutions meeting the preferences of the DM and not many other solutions, one may consider them as computationally efficient. Time and effort from the DM are continually required, which may not always be practicable. The full range of Pareto optimal solutions may not be available.

Selected MOO methods are described in detail in later chapters of this book. Here, the weighting method and the ε -constraint method will be briefly described. These two classical methods have been used for solving several chemical engineering applications. Interestingly, a few studies reported in the literature have used the weighting or ε -constraint method without explicitly referring MOO. For example, Therdthai *et al.* (2002) optimized the bread oven temperature to minimize the weight loss during baking, for several values of baking times. Obviously, it is desirable to reduce the baking time, which is thus the second objective but considered as a constraint in Therdthai *et al.* (2002).

For solving the MOO problem in equation 1.1 by the weighting method, it is converted into the following SOO problem:

$$\text{Minimize} \quad w \frac{f_1(\mathbf{x}) - f_1^*}{f_1^N - f_1^*} + (1-w) \frac{f_2(\mathbf{x}) - f_2^*}{f_2^N - f_2^*} \quad (1.2)$$

with respect to \mathbf{x} subject to the bounds and constraints in equations 1.1(c) to 1.1(e). Here, $0 \leq w \leq 1$ is the weighting factor. Recall that the superscript * and N refer to the ideal and nadir objective vector respectively. These vector components are used for normalizing the objectives, which are likely to have significantly different magnitudes in applications. Although it is possible to define the objective in equation 1.2 without the normalizing factors, the solution of the resulting SOO problem will depend on w to a greater extent. The optimization problem in equation 1.2 will have to be solved several times, each time with a different w , in order to find several Pareto-optimal solutions. Note that $w = 1$ corresponds to minimizing $f_1(\mathbf{x})$ by itself whereas $w = 0$ correspond to minimizing $f_2(\mathbf{x})$ alone. Even though the weighting method is conceptually straightforward, choosing suitable w to find many Pareto-optimal solutions is difficult.

In the ε -constraint method, the MOO problem is transformed into a SOO problem by retaining only one of the objectives and converting all others into inequality constraints. For example, the MOO problem in equation 1.1 is transformed as:

$$\text{Minimize} \quad f_2(\mathbf{x}) \quad (1.3)$$

with respect to \mathbf{x} subject to the bounds and constraints in equations 1.1(c) to 1.1(e) as well as an additional constraint: $f_1(\mathbf{x}) \leq \varepsilon$. Here, the second objective, $f_2(\mathbf{x})$ is retained but the objective, $f_1(\mathbf{x})$ is included as an inequality constraint such that its value is not more than ε at the optimal solution of the problem in equation 1.2. Obviously, the user will have to

select which objective to be retained and the value of ε . The problem in equation 1.3 will have to be solved for a range of ε values in order to find many Pareto-optimal solutions. The difficulties in the ε -constraint method are selection of ε value and solving the problem in equation 1.3. The additional constraint in this problem makes it more difficult to solve. Further, the SOO problem in the ε -constraint method may not have a feasible solution for some ε values. Values of the ideal and nadir objective vectors can be used for selecting suitable ε values.

1.4 Alkylation Process Optimization for Two Objectives

An important process in petroleum refining is the alkylation process, wherein a light olefin such as propene, butene or pentene reacts with isobutane in the presence of a strong sulfuric acid catalyst to produce the alkylate product (e.g., 2,2,4 tri-methyl pentane from butene and isobutane). The alkylate product is used for blending with refinery products such as gasoline and aviation fuel in order to increase their Octane Number. Jones (1996) provides a comprehensive overview of the alkylation process, its chemistry, design and operational aspects. Sauer *et al.* (1964) developed a nonlinear model for the alkylation process and used it for optimization via linear programming methods. Since then, many researchers (e.g., Bracken and McCormick, 1968; Luus and Jaakola, 1973; Rangaiah, 1985) employed this model in their optimization studies. Also, alkylation process optimization is a classic example included in the text-book on optimization by Edgar *et al.* (2001). To the best of our knowledge, only Luus (1978) reported alkylation process optimization for multiple objectives by the ε -constraint method; for this optimization, he modified the bounds on variables slightly compared to those in Sauer *et al.* (1964). Here, we will describe optimization of the alkylation process for two objectives by the ε -constraint method.

1.4.1 Alkylation Process and its Model

A simplified process flow diagram of the alkylation process is shown in Figure 1.4. The process has a reactor with olefin feed, isobutane makeup and isobutane recycle as the inlet streams. Fresh acid is added to catalyze the reaction and spent acid is withdrawn. The exothermic

reactions between olefins and isobutane occur at around room temperature, and excess isobutane is used. The hydrocarbon outlet stream from the reactor is fed into a fractionator from where isobutane is recovered at the top and recycled back to the reactor, and the alkylate product is withdrawn from the bottom.

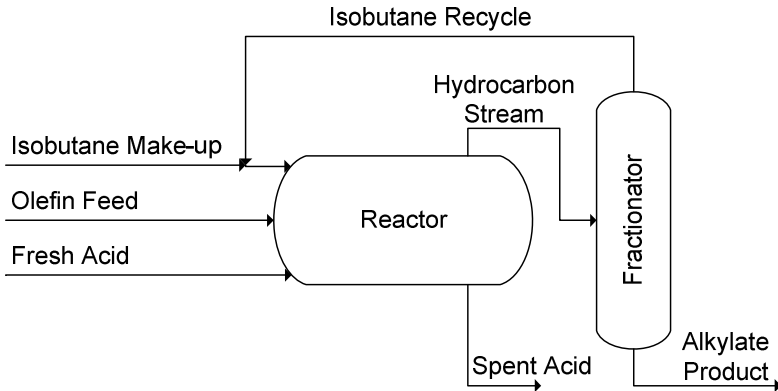


Fig. 1.4 Simplified schematic of the alkylation process.

Sauer *et al.* (1964) developed a model for this process based on a judicious combination of first principles, empirical equations and a number of simplifying assumptions. The resulting model has 10 variables and seven equality constraints. Bracken and McCormick (1968) have presented this model and the optimization problem in a different way. Noting that the four equality constraints derived by regression analysis need not be satisfied exactly, they converted them into eight inequality constraints. This optimization problem and its solution are concisely described by Edgar *et al.* (2001). Rangaiah (1985) studied both the problems - original one with seven equality constraints and the modified one with both equality and inequality constraints.

Variables involved in the alkylation process model of Sauer *et al.* (1964) and their bounds are summarized in Table 1.2. The SOO problem of this process is as follows.

$$\begin{aligned} \text{Maximize} \quad & \text{Profit, } P \text{ (\$/day)} = 0.063 x_4 x_7 - 5.04 x_1 - 0.035 x_2 \\ & - 10.0 x_3 - 3.36 x_5 \end{aligned} \quad (1.4a)$$

With respect to x_1, x_7 and x_8

$$\text{Subject to} \quad 0 \leq x_1 \leq 2,000 \quad (1.4b)$$

$$90 \leq x_7 \leq 95 \quad (1.4c)$$

$$3 \leq x_8 \leq 12 \quad (1.4d)$$

$$0 \leq [x_4 \equiv x_1(1.12 + 0.13167x_8 - 0.006667x_8^2)] \leq 5,000 \quad (1.4e)$$

$$0 \leq [x_5 \equiv 1.22x_4 - x_1] \leq 2,000 \quad (1.4f)$$

$$0 \leq [x_2 \equiv x_1 x_8 - x_5] \leq 16,000 \quad (1.4g)$$

$$85 \leq [x_6 \equiv 89 + (x_7 - (86.35 + 1.098x_8 - 0.038x_8^2))/0.325] \leq 93 \quad (1.4h)$$

$$145 \leq [x_{10} \equiv -133 + 3x_7] \leq 162 \quad (1.4i)$$

$$1.2 \leq [x_9 \equiv 35.82 - 0.222x_{10}] \leq 4 \quad (1.4j)$$

$$0 \leq [x_3 \equiv 0.001(x_4 x_6 x_9)/(98 - x_6)] \leq 120 \quad (1.4k)$$

The above problem will be referred to as Problem A in the following. The 7 inequality constraints in equations 1.4e to 1.4k are the bounds on the 7 variables (x_4 , x_5 , x_2 , x_6 , x_{10} , x_9 and x_3) in the original problem, and they arise from the elimination of these variables from the 7 equality constraints in the model thus making them dependent variables. The cost coefficients in the profit are alkylate product value (\$0.063/octane-barrel), olefin feed cost (\$5.04/barrel), isobutane recycle cost (\$0.035/barrel), fresh acid cost (\$10.0/thousand pounds) and isobutane feed cost (\$3.36/barrel). The optimal solution for this SOO problem is also presented in Table 1.2. The reader can verify this using the Excel file: "Alkylation.xls" in the folder: Chapter 1 on the compact disk (CD) provided with the book.

Table 1.2 Variables, Bounds and Optimum Values in the Alkylation Process Optimization

Variables	Lower Bound	Upper Bound	Optimum Value
Olefin Feed, x_1 (barrels/day)	0	2,000	1,728
Isobutane Recycle, x_2 (barrels/day)	0	16,000	16,000
Acid Addition Rate, x_3 (thousand pounds/day)	0	120	98.14
Alkylate Production Rate, x_4 (barrels/day)	0	5,000	3,056
Isobutane Feed, x_5 (barrels/day)	0	2,000	2,000
Spent Acid Strength, x_6 (weight percent)	85	93	90.62
Octane Number, x_7	90	95	94.19
Isobutane to Olefin Ratio, x_8	3	12	10.41
Acid Dilution Factor, x_9	1.2	4	2.616
F-4 Performance Number, x_{10}	145	162	149.6
Profit (\$/day)			1,162

1.4.2 Multi-Objective Optimization Results and Discussion

The SOO problem (Problem A) can be formulated as a two-objective problem by adding another objective. We consider two such problems:

Case A - Maximize Profit, P and Maximize Octane Number, x_7

Case B - Maximize Profit, P and Minimize Isobutane Recycle, x_2

Alkylate product with a higher octane number is better for blending with refinery products. Minimizing isobutane recycle helps to reduce fractionation and other costs associated with the recycle stream.

The ε -constraint method can be easily applied to solve both the two-objective problems since one objective (x_7 or x_2) is a variable whose range is known from the problem formulation. For this, the SOO problem for Case A is the same as Problem A except for the change in the lower bound of x_7 to ε (i.e., desired lowest value for the second objective) instead of 90. Since the optimum x_7 in Problem A is at 94.19, the solution of Case A by the ε -constraint for $\varepsilon \leq 94.19$ will be the same as that in Table 1.2. The Pareto-optimal solutions of Case A obtained by the ε -constraint method for several values of ε in the range 94.2 to 95.3 are presented in Figure 1.5. These and other results for the alkylation process optimization were obtained using the Solver tool in Excel. Note that the upper bound of x_7 will have to be changed for higher values of ε in order to have feasible region satisfying all bounds and constraints. Further, no feasible solution exists for ε above 95.3, which is understandable since the model is semi-empirical.

In Figure 1.5, the first plot shows the two objectives (P on the x-axis and x_7 on the y-axis) and the remaining plots show the optimal values of all other decision variables versus P. Increase in P from 1,000 to 1,106 \$/day is accompanied by x_7 decreasing from 95.3 to 94.3; thus, the two objectives, P and x_7 are contradictory leading to the optimal Pareto front in the first plot in Figure 1.5. All other decision variables with the exception of x_2 (isobutane recycle) which remains at its upper bound, contribute to the optimal Pareto front. Interestingly, each of them varies with P at certain rate until P is about \$1,110/day and then follows a different trend - x_1 , x_4 , x_5 and x_8 become constant, x_3 and x_6 start to decrease at $P > \$1,110/\text{day}$. Of these, the trend of x_3 is striking - it increases with P initially and then decreases for $P > \$1,110/\text{day}$.

In a similar way, the two-objective problem in Case B can also be solved by the ε -constraint method; the corresponding SOO problem is the same as Problem A except that the upper bound on x_2 (which is an

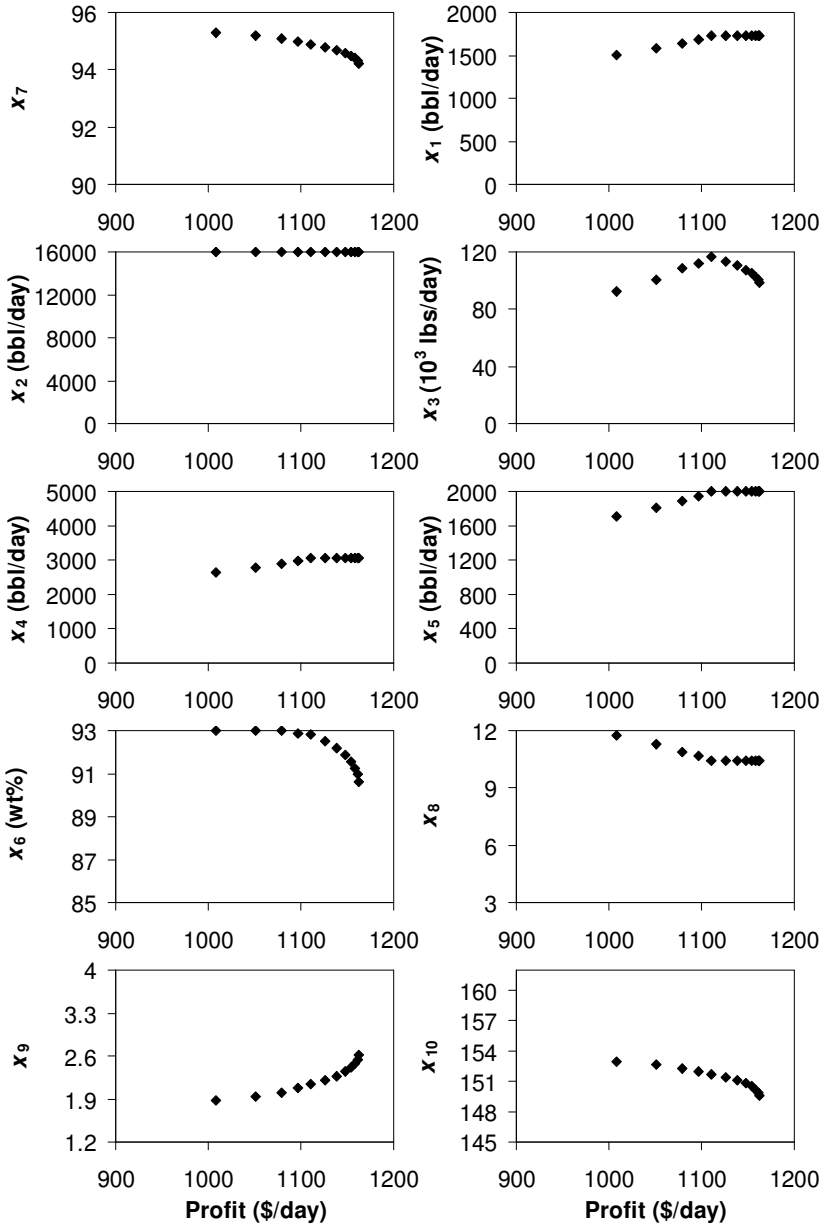


Fig. 1.5 Pareto-optimal solutions for maximizing profit and octane number (x_7) by the ϵ -constraint method; profit is shown on the x-axis in all plots.

inequality constraint in Problem A) is the ε . Pareto-optimal solutions resulting from solving a series of such SOO problems with ε in the range 12,000 to 17,500 barrels/day are shown in Figure 1.6. The optimal P increases from about 900 to 1,200 \$/day as x_2 increases from 12,000 to 17,500 barrels/day. As in Case A, the two objectives – maximize P and minimize x_2 , are contradictory. In Case B, all decision variables contribute to the optimal Pareto front and none of them is constant over the range of P shown in Figure 1.6. Similar to Case A, each of the decision variables show certain trend up to P = \$1,050/day and then a different trend. Interestingly, x_3 increases with P initially and then starts decreasing beyond P = \$1,050/day. Further, optimal values of decision variables in Case B are generally different from those in Case A.

Although an experienced engineer may be able to predict some trends of objectives and decision variables in Figures 1.5 and 1.6, it is impossible to foretell them accurately and correctly. On the other hand, MOO can give many optimal solutions, which in turn provide greater insight into and understanding of the process behavior. Knowing these solutions, their trends and additional considerations, the most suitable optimal solution can then be selected for implementation. The two-objective problem in Cases A can also be solved by the weighting method; this is given as an exercise at the end of this chapter.

1.5 Scope and Organization of the Book

This book, as implied by its title, focuses on both MOO techniques and their applications in chemical engineering. The chapters in the book can be divided into three groups. The first group consists of this introduction chapter and another chapter summarizing the MOO applications in chemical engineering reported from the year 2000 to mid 2007. The second group of 5 chapters is on the MOO techniques written by leading researchers in the field. The last group of 6 chapters is on a broad range of MOO applications in chemical engineering including a few on biochemical engineering. Each of the chapters in the book can be read and understood with little reference to other chapters. Many chapters contain several exercises at the end; these and the applications discussed within the chapters can be used as projects and/or assignments in optimization courses at both undergraduate and postgraduate levels. The programs and files on the enclosed CD will be helpful to readers in solving the exercises and/or doing the projects.

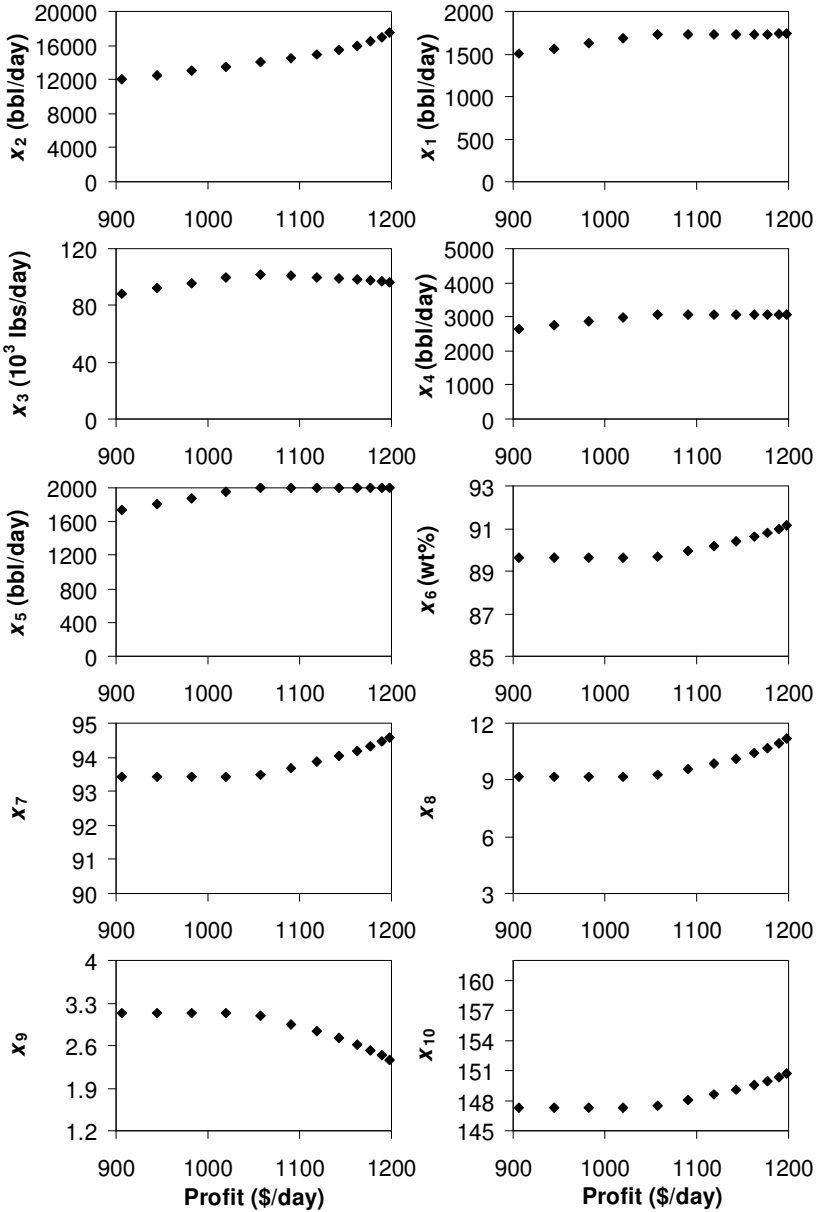


Fig. 1.6 Pareto-optimal solutions for maximizing profit and isobutane recycle (x_2) by the ϵ -constraint method; profit is shown on the x-axis in all plots.

Nearly 100 MOO applications in chemical engineering reported in journals from the year 2000 until mid 2007 are summarized by Masuduzzaman and Rangaiah in Chapter 2: *MOO Applications in Chemical Engineering*. These applications are categorized into five groups: (1) process design and operation, (2) biotechnology and food industry, (3) petroleum refining and petrochemicals, (4) pharmaceuticals and other products/processes, and (5) polymerization. However, the applications reported in this book are not included in this review. Many applications reviewed in Chapter 2 have employed detailed models of the processes for their optimization for a variety of objectives. Several others have used process simulators in their studies. Thus, Chapter 2 is a very rich source of reported MOO applications in chemical engineering as well as process models for many processes of importance.

In Chapter 3 entitled *Multi-objective Evolutionary Algorithms: A Review of the State-of-the-Art and some of their Applications in Chemical Engineering*, Jaimes and Coello Coello review development of evolutionary algorithms for MOO and some of their applications in chemical engineering. They also identify several contributions of chemical engineering researchers to the development of multi-objective evolutionary algorithms (MOEAs). Towards the end of the chapter, Jaimes and Coello Coello list available resources including websites and public-domain software on MOEAs, and then outline potential areas for future research on the use of MOEAs in chemical engineering.

Ramteke and Gupta, in Chapter 4: *The Jumping Gene Adaptations of Multi-objective Genetic Algorithm and Simulated Annealing*, describe genetic algorithms and simulated annealing, first for SOO, then for MOO and finally their jumping gene adaptations. The presented algorithms are tested on a few benchmark problems; the results are presented and discussed. Incorporating the macro-macro mutation operation, namely, jumping gene operator inspired from nature, leads to faster convergence of the algorithm. Towards the end of the chapter, Ramteke and Gupta review their more recent chemical engineering applications of the jumping gene adaptations of genetic algorithm and simulated annealing.

In Chapter 5 entitled *MOO using Surrogate Assisted Evolutionary Algorithm*, Ray describes a surrogate-assisted evolutionary algorithm for MOO in order to reduce the number of objective function and constraint evaluations. In this algorithm, a radial basis function (RBF) neural network is used as a surrogate/approximate model for the objectives and constraints, for certain number of generations instead of the original

objective functions and constraints before developing a new surrogate model. The results on several test functions show that the surrogate-assisted evolutionary algorithm provides better non-dominated solutions than the elitist non-dominated sorting genetic algorithm (NSGA-II) for the same number of actual function and constraint evaluations. This is particularly advantageous in chemical engineering applications which involve computationally-intensive process simulation for evaluating the objectives and/or constraints.

Chapter 6: *Why Use Interactive MOO in Chemical Process Design?* by Miettinen and Hakanen focuses on problems having several (i.e., more than 2) objective functions and interactive MOO. They describe weighting method, ε -constraint method and evolutionary MOO methods, their relative merits, and then a few interactive MOO methods including their NIMBUS method and its two implementations. In the later part of the chapter, Miettinen and Hakanen discuss the application of interactive MOO methods to chemical process design. Application of the NIMBUS method is then illustrated for optimizing a simulated moving bed process for separation of fructose and glucose for four objectives. Two other applications, namely, water allocation problem having three objectives and heat recovery system design with four objectives, are also outlined.

Many studies on MOO applications in chemical engineering focus on generating Pareto-optimal solutions. The important step of ranking these solutions is the subject of Chapter 7: *Net Flow and Rough Set: Two Methods for Ranking the Pareto Domain* by Thibault. In this chapter, net flow and rough sets methods for ranking Pareto-optimal solutions are described in detail. Both the methods require the preferences and knowledge of the decision maker. A few variants of rough sets method are also discussed. In the later part of the chapter, net flow and rough set methods are applied for ranking Pareto-optimal solutions for optimization of gluconic acid production for two, three and four objectives. The results obtained are presented and discussed.

In Chapter 8: *MOO of Gas Phase Refrigeration Systems for LNG*, Shah, Rangaiah and Hoadley describe the optimization of multi-stage gas-phase refrigeration systems for capital cost and energy efficiency simultaneously, for the first time. They employed a process simulator (namely, Hysys) for simulation, NSGA-II for MOO and an interface program for linking Hysys and NSGA-II. Design and optimization of two multi-stage gas-phase refrigeration systems (one for nitrogen cooling and another for liquefaction of natural gas) are discussed in detail.

Optimization of feed to an industrial fluidized catalytic cracker (FCC) important in petroleum refining, is the application described by Tan, Phang and Yang in Chapter 9 entitled *A Multi-objective Evolutionary Algorithm for Practical Residue Catalytic Cracking Feed Optimization*. In this particular refinery, there are seven different feed streams, each with its own flow range and characteristics, which can be used for the FCC. The feed optimization problem consists of three objectives subject to four constraints. It is solved using a multi-objective optimization evolutionary algorithm (MOEA) toolbox, and Pareto-optimal solutions are presented. Of particular interest in this application is the analysis and discussion on selecting a Pareto-optimal solution for implementation based on three performance indexes: fuel gas consumption, steam consumption and exothermic reaction rate.

Lee, Rangaiah and Agrawal report the optimization of three applications for multiple economic and/or environmental objectives using NSGA-II-aJG, in Chapter 10: *Optimal Design of Chemical Processes for Multiple Economic and Environmental Objectives*. The first two applications are the optimization of the classical Williams-Otto process and the optimal design of a low density polyethylene plant, both for two economic objectives simultaneously. Results of these two applications show that some economic criteria could be conflicting depending on the model equations and objectives. The third application is on the optimization of industrial ecosystems consisting of several plants for both economic and environmental criteria. As expected, the economic and environmental criteria are found to be conflicting leading to Pareto-optimal solutions for industrial ecosystem optimization.

An interesting application of MOO to emergency response around chemical plants is described by Georgiadou, Papazoglou, Kiranoudis and Markatos in Chapter 11 entitled *Multi-objective Emergency Response Optimization around Chemical Plants*. Problem formulation for emergency response optimization and an MOEA are described. They are then applied to two case studies: emergency response optimization for accidental ammonia release from a storage tank and for BLEVE (boiling liquid expanding vapor explosion) in a petroleum refinery. The results of MOO are presented and their use for emergency planning and land-use planning is highlighted.

The penultimate chapter: *Array Informatics using Multi-objective Genetic Algorithms: From Gene Expressions to Gene Networks* by Garg is on elucidating gene networks from microarray experimental data. This

application area is new to many chemical engineers. Hence, the chapter begins with a detailed introduction covering biological background, multiple microarray experiments to measure gene expressions¹ of several hundreds of genes, interpreting and pre-processing microarray data. The measured expression ratios are first analyzed to identify groups of genes with similar ratios via clustering techniques; the results of this step (known as gene expression profiling) are then used to model the complex interactions among genes (which is referred to as gene network analysis). MOO is applicable to both gene expression profiling and network analysis. This is successfully illustrated on two gene expression data sets: a synthetic data set and a real-life data set, to find the gene networks.

The last chapter entitled *Optimization of a multi-product microbial cell factory for multiple objectives – a paradigm for metabolic pathway recipe*, by Lee, Rangaiah and Lee reports a novel application of MOO to metabolic engineering. They present the optimization of gene manipulation (knockout, overexpression or repression) for two objectives in order to optimize production of desired amino acids by *Escherichia coli* (*E. coli*). The mixed-integer MOO problem in this application was successfully solved using the NSGA-II; this was particularly facilitated by the possibility of continuous and/or integer variables within NSGA-II. The MOO results show that fluxes of desired enzymes can be increased significantly by optimal manipulation of just three enzymes.

References

- Beveridge, G. S. G. and Schechter, R. S. (1970). *Optimization: Theory and Practice*, McGraw Hill, New York.
- Bhaskar, V., Gupta, S. K. and Ray, A. K. (2000). Applications of multi-objective optimization in chemical engineering, *Reviews in Chemical Engineering*, 16, pp. 1-54.
- Biegler, L. T., Grossmann, I. E. and Westerberg, A. W. (1997). *Systematic Methods of Chemical Process Design*, Prentice Hall, New Jersey.
- Bracken, J. and McCormick, G. P. (1968). *Selected Applications of Nonlinear Programming*, John Wiley, New York.
- Chankong, V. and Haimes, Y. Y. (1983). *Multi-objective Decision Making Theory and Methodology*, Elsevier Science Publishing, New York.
- Coello Coello, C. A., Veldhuizen, D. A. V. and Lamont, G. B. (2002). *Evolutionary Algorithms for Solving Multi-objective Problems*, Kluwer Academic, New York.

¹Gene expression is the process by which the set of instructions is read by the cell and translated into proteins.

- Cohon, J. L. (1978). *Multi-objective Programming and Planning*, Academic Press, New York.
- Deb, K. (2001). *Multi-objective Optimization Using Evolutionary Algorithms*, Wiley, Chichester, UK.
- Diwekar, U. M. (2003). *Introduction to Applied Optimization*, Kluwer Academic, Norwell, Mass.
- Edgar, T. F., Himmelblau, D. M. and Lasdon, L. S. (2001). *Optimization of Chemical Processes*, Second Edition, McGraw-Hill, New York.
- Floudas, C. A. (1995). *Nonlinear Mixed-integer Optimization: Fundamentals and Applications*, Oxford University Press, New York.
- Floudas, C. A. (1999). *Deterministic Global Optimization: Theory, Methods and Applications*, Kluwer Academic, Boston.
- Haimes, Y. Y., Tarvainen, K., Shima, T. and Thadathil, J. (1990). *Hierarchical Multi-objective Analysis of Large-Scale Systems*, Hemisphere Publishing, New York.
- Himmelblau, D. M. (1972). *Applied Nonlinear Programming*, McGraw-Hill, New York.
- Hwang, C. L. and Masud, A. S. M. (1979). *Multiple Objective Decision Making - Methods and Applications: A State-of-the-Art Survey*, Springer-Verlag, Lecture Notes in Economics and Mathematical Systems, Berlin.
- Jones, D. S. J. (1996). *Elements of Petroleum Processing*, Chapter 14, John Wiley, New York.
- Lapidus, L. and Luus, R. (1967). *Optimal Control in Engineering Processes*. Blaisdell, Waltham, Mass.
- Luus, R. (2000). *Iterative Dynamic Programming*, Chapman & Hall, Boca Raton.
- Luus, R. and Jaakola, T. H. I. (1973). Optimization by direct search and systematic reduction of the size of search region. *AIChE Journal*, 19, pp. 760-766.
- Luus, R. (1978). Optimization of systems with multiple objective functions. *International Congress, European Federation of Chemical Engineering*, Paris, pp. 3-8.
- Miettinen, K. (1999). *Nonlinear Multi-objective Optimization*, Kluwer Academic Publishers, Boston.
- Peters, M. S., Timmerhaus, K. D. and West, R. E. (2003). *Plant Design and Economics for Chemical Engineers*, McGraw-Hill, Boston.
- Ray, W. H. and Szekely, J. (1973). *Process Optimization with Applications in Metallurgy and Chemical Engineering*, Wiley, New York.
- Rangaiah, G. P. (1985). Studies in constrained optimization of chemical processes. *Computers and Chemical Engineering*, 9, pp. 395-404.
- Reklaitis, G. V., Ravindran, A. and Ragsdell, K. M. (2006). *Engineering Optimization: Methods and Applications*, Second Edition, John Wiley, New Jersey.
- Sauer, R. N., Colville, Jr., A. R. and Burwick, C. W. (1964). Computer Points the Way to More Profits, *Hydrocarbon Processing & Refiner*, 49, No. 2, pp. 84-92.
- Sawaragi Y., Nakayama, H. and Tanino, T. (1985). *Theory of Multi-objective Optimization*, Academic Press, Orlando, Florida.
- Seider, W. D., Seader, J. D. and Lewin, D. R. (2003). *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*, John Wiley, New York.
- Stadler, W. (1988). *Multi-criteria Optimization in Engineering and in the Sciences*, Plenum Press, New York.
- Tan, K. C., Khor, E. F. and Lee, T. H. (2005). *Multi-objective Evolutionary Algorithms and Applications*, Springer, London.

- Tarafder, A., Rangaiah, G. P. and Ray, A. K. (2007). A Study of Finding Many Desirable Solutions in Multi-objective Optimization of Chemical Processes. *Computers and Chemical Engineering*, 31, pp. 1257-1271.
- Tawarmalani, M. and Sahinidis, N. V. (2002). *Convexification and Global Optimization in Continuous and Mixed-integer Nonlinear Programming: Theory, Algorithms, Software and Applications*, Kluwer Academic, Dordrecht.
- Therdthai, N. Zhou, W. and Adamczak, T. (2002). Optimization of the temperature profile in bread baking, *Journal of Food Engineering*, 55, pp. 41-48.
- Weistroffer, H. R. (1985). Careful usage of pessimistic values is needed in multiple objectives optimization, *Operations Research Letters*, 4, pp. 23-25.

Exercises

- 1.1 Identify a daily-life situation (e.g., selection of a course of study, job and investment) requiring selection. What are the choices available? What are the objectives to be achieved? Are one or more objectives conflicting in nature? What are the constraints? Discuss these and any other related issues qualitatively. State the information and/or relations required if the optimization problem has to be solved quantitatively.
- 1.2 Optimize the alkylation process for two objectives (cases A and/or B) using the ϵ -constraint method and Solver tool in Excel. Are the results comparable to those in Figures 1.5 and 1.6?
- 1.3 Optimize the alkylation process for two objectives (cases A and/or B) using the weighting method. One can use the Solver tool in Excel for SOO. Try different weights to find as many Pareto-optimal solutions as possible. Compare and comment on the solutions obtained with those obtained by the ϵ -constraint method (Figures 1.5 and 1.6). Which of the two methods – the weighting and the ϵ -constraint method, is better?
- 1.4 Optimize the alkylation process for two objectives (cases A and/or B) using a MOO program (e.g., see Chapters 4 and 5 for two programs provided on the attached CD). Note the computational time taken for each of the two cases. Compare the results obtained with those presented in this chapter. Also, optimize the alkylation process for three objectives: maximize profit, maximize octane number and minimize isobutene recycle, using the same program. Compare and discuss the results obtained with those for cases A and B. Does three-objective optimization require comparable or more computational time than two-objective optimization?