Part I
Overview

Multi-Objective Optimization in Chemical Engineering: Developments and Applications, First Edition.
Edited by Gade Pandu Rangaiah and Adrián Bonilla-Petriciolet.
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Introduction

Adrián Bonilla-Petriciolet[1] *and Gade Pandu Rangaiah*[2]
[1]*Department of Chemical Engineering, Instituto Tecnológico de Aguascalientes, Aguascalientes, Mexico*
[2]*Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore*

1.1 Optimization and Chemical Engineering

Optimization is important for process modeling, synthesis, design, operation and retrofitting of chemical, petrochemical, pharmaceutical, energy and related processes. Usually, chemical engineers need to optimize the design and operating conditions of industrial process systems to improve their performance, costs, profitability, safety and reliability. Process system optimization is challenging because chemical engineering application problems are often complex, nonlinear and large, have both equality and inequality constraints and/or involve both continuous and discrete decision variables. The mathematical relationships among the objective to be optimized (also known as the performance criterion), constraints and decision variables establish the difficulty and complexity of the optimization problem, as well as the optimization method that should be used for its solution. In particular, the type of search space (i.e., continuous or discrete), the properties of the objective function (e.g., convex or non-convex, differentiable or nondifferentiable), and the presence and nature of constraints (e.g., equality or inequality, linear or nonlinear) are the principal characteristics to classify an optimization problem (Biegler and Grossmann, 2004).

The classes of optimization problems commonly found in engineering applications include linear programming, quadratic programming, nonlinear programming, combinatorial optimization, dynamic optimization, mixed integer linear/nonlinear programming, optimization under uncertainty, bi-level optimization, global optimization and multi-objective

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optimization (Floudas, 2000; Diwekar, 2003; Biegler and Grossmann, 2004; Floudas *et al.*, 2005). These types of optimization problems are found in almost all application areas such as modeling, synthesis, design, operation and control of chemical and related processes, and a wide variety of numerical methods have been used to solve them (e.g., Luus, 2000; Edgar *et al.*, 2001; Tawarmalani and Sahinidis, 2002; Diwekar, 2003; Biegler and Grossmann, 2004; Grossmann and Biegler, 2004; Floudas *et al.*, 2005; Ravindran *et al.*, 2006; Rangaiah, 2009 and 2010).

Application problems may have multiple optima, and it may be essential to find the global optimum or the best solution. Depending on their convergence properties, optimization methods can be classified as local or global. They may also be classified as deterministic or stochastic methods depending on whether their search is deterministic (often using gradient of the objective function and other properties of the problem) or stochastic (employing random numbers). Local methods are computationally efficient and suitable for finding a local optimum. These search strategies have been exploited commercially as can be seen from their implementation in common software and process simulators such as Solver tool in Excel, optimization tool-box in Matlab, GAMS, Aspen Plus and Hysys. Current progress in computational capabilities has prompted an increasing and considerable attention on the incorporation of global optimization methods in commercial software. For example, an evolutionary search engine is now available in the Solver tool. Global methods are more likely to find the global optimum.

To date, research contributions in optimization for chemical engineering have focused primarily on theoretical and algorithmic advances including the development of reliable and efficient strategies and their application for solving challenging and important chemical engineering problems. The majority of these contributions deal with optimization problems having only one objective function. In general, optimization problems in chemical engineering and in other disciplines involve more than one objective function related to performance, economics, safety and reliability, which have to be optimized simultaneously since these objective functions may be fully or partially conflicting over the range of interest. Examples of conflicting objectives are: capital investment versus operating cost; cost versus safety; quality versus recovery/cost; and environmental impact versus profitability. Multi-objective optimization (MOO), also known as multi-criteria optimization, is necessary to find the optimal solution(s) in the presence of tradeoffs among two or more conflicting objectives.

Multi-objective optimization has therefore been studied and applied to solve a variety of challenging and important problems in chemical engineering (Bhaskar *et al.*, 2000; Rangaiah, 2009; Chapter 3 in this book). In a perspective paper on issues and trends in the teaching of process and product design, Biegler *et al.* (2010) noted that an important goal in process design is optimization for multiple objectives such as profit, energy consumption and environmental impact. In another perspective paper on sustainability in chemical engineering education, identifying a core body of knowledge, Allen and Shonnard (2012) have included process optimization as one of the computer-aided tools for environmentally-conscious design of chemical processes; within process optimization, they have listed multi-objective, mixed integer and nonlinear optimization. Both these perspectives from eminent researchers attest the growing importance and need for MOO in chemical engineering.

Even though research in the application of MOO in engineering has grown significantly, there is only one book specifically devoted to MOO techniques and their applications

in chemical engineering (Rangaiah, 2009); it describes selected MOO techniques and discusses many applications. MOO and its applications are growing with new developments and interesting applications being reported continually. The present book covers the most recent developments in MOO methods and novel applications of MOO for modeling, design and operation of chemical, petrochemical, pharmaceutical, energy and related processes. In short, the present book complements the previous book on MOO in chemical engineering. The remainder of this chapter is organized as follows. Section 1.2 provides the basic concepts and definitions used in MOO. Section 1.3 discusses MOO briefly in the context of chemical engineering. Finally, section 1.4 presents an overview of all the chapters in this book.

1.2 Basic Definitions and Concepts of Multi-Objective Optimization

In this section, basic definitions and key concepts in MOO are introduced briefly. The reader is referred to earlier publications (e.g., Deb, 2001; Coello Coello *et al.*, 2002; Rangaiah, 2009) for more details on these topics. Formally, MOO refers to simultaneous optimization (i.e., maximization and/or minimization) of two or more objective functions, which are often in conflict with one another. This optimization problem can be stated as follows:

$$Optimize \langle f_1(\boldsymbol{x}),\ f_2(\boldsymbol{x}), \ldots,\ f_n(\boldsymbol{x})\rangle \tag{1.1}$$

subject to

$$\begin{aligned} & g_i(\boldsymbol{x}) \le 0 \quad i = 1, 2, \ldots, n_i \\ & h_i(\boldsymbol{x}) = 0 \quad i = 1, 2, \ldots, n_e \\ & \boldsymbol{x_l} < \boldsymbol{x} < \boldsymbol{x_u} \end{aligned} \tag{1.2}$$

where n is the number of objective functions to be simultaneously optimized, $\boldsymbol{x}$ is the vector of m decision variables (continuous and/or discontinuous) with lower ($\boldsymbol{x_l}$) and upper ($\boldsymbol{x_u}$) bounds, n_i and n_e are the number of inequality (g) and equality (h) constraints, respectively. The feasible space, F is the set of vectors $\boldsymbol{x}$ that satisfy all the constraints and bounds in Equation 1.2.

In MOO, we are interested in determining the set of values of $\boldsymbol{x}$ that yields the best compromise solutions for all the specified objective functions. A single solution that simultaneously optimizes conflicting objectives is not feasible. Instead, a set of solutions is found with the following characteristic: improvement of any one of the objectives is not possible without worsening one or more of other objectives in the optimization problem. These optimal solutions are referred to as the Pareto-optimal solutions (named after Italian economist, Vilfredo Pareto). They provide quantitative tradeoffs among the objectives involved.

A vector $\boldsymbol{x}^* \in F$ is Pareto optimal if there exists no feasible vector $\boldsymbol{x} \in F$ that would improve some objective function without causing a simultaneous deterioration in at least one other objective function. The Pareto-optimal solutions are also called non-dominated solutions. In this context, the concept of domination implies that, given two solutions S1 and S3, S1 dominates S3 if S1 is at least as good as S3 in all objectives and better in at least one (see Figure 1.1(a)). If neither of the solutions dominates the other, then both are non-dominated to each other (e.g., S1 and S2 in Figure 1.1(a)). The determination of the

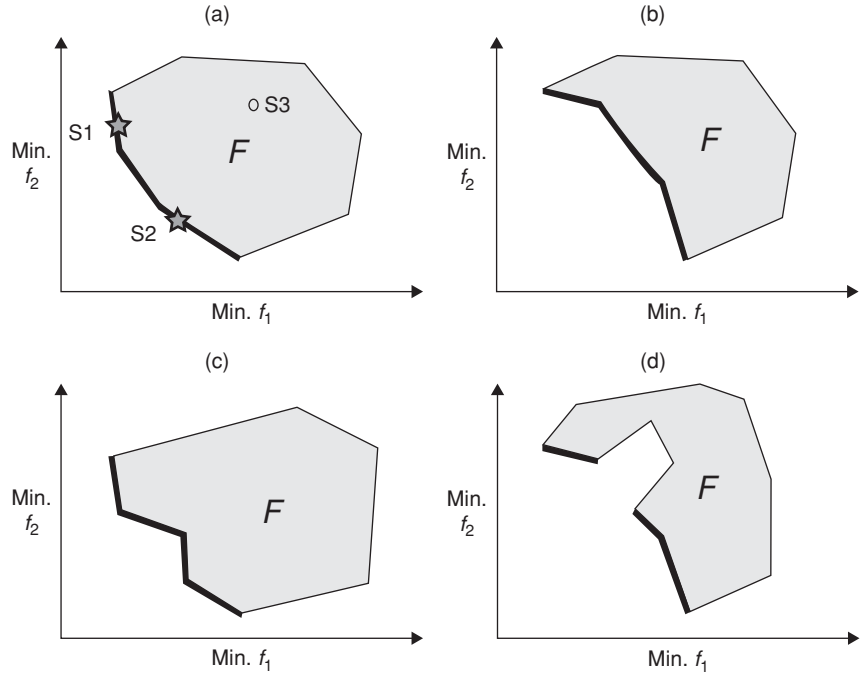

Figure 1.1 *Possible Pareto-optimal fronts for bi-objective optimization: (a) convex, (b) concave, (c) concave and convex and (d) disconnected front. Gray region is the feasible space, and the thick edge is the Pareto-optimal front.*

Pareto-optimal front (i.e., the set of non-dominated solutions) is the main goal in MOO. A process engineer can establish and understand tradeoffs and process performance using the MOO results. The selection of a solution from the Pareto-optimal front depends on the decision maker's preferences, knowledge about the studied problem and also optimal values of decision variables. Therefore, the decision maker, based on his/her expertise and intuition, needs to choose the most appropriate solution for implementation or particular regions of the tradeoff surface for further exploration.

In general, a good Pareto-optimal front should show two desirable characteristics: the non-dominated solutions are distributed evenly, and they cover a wide range of values of objectives under study. However, finding such a Pareto-optimal front can be very difficult especially for large problems with non-continuous and non-convex search spaces. In MOO, the concept of a local minimum is replaced by a local Pareto-optimal front, whose presence may cause problems in the convergence of MOO methods to the global Pareto-optimal front.

The Pareto-optimal fronts can be concave, convex or may consist of both concave and convex sections including discontinuities. Figure 1.1 illustrates these for the case of a bi-objective optimization problem. Better non-dominated solutions are obtained by MOO methods for problems having convex Pareto fronts than for those having concave Pareto fronts. The Pareto-optimal fronts with discontinuities are common in engineering problems,

and are more complex to analyze. The problem dimension can affect the size and shape of the Pareto-optimal set, and consequently determines the performance of MOO methods. Further, the complexity of and difficulty of solving multi-objective problems as well as the difficulty of analyzing their solutions are likely to increase with number of objectives.

There are several types of algorithms used for solving MOO problems to find the Pareto-optimal solutions (Miettinen, 1999; Rangaiah, 2009). These include different types of weighted methods (e.g., global criterion, weighted sum, weighted min-max, weighted product, exponential weighted), goal programming methods, the bounded objective function method, the ε-constraint method, meta-heuristic/stochastic methods (Coello Coello *et al.*, 2002; Marler and Arora, 2009). Methods to solve MOO problems can be classified in different ways, for example, depending on the decision-maker's preference (i.e., methods with a priori, posteriori and without articulation of preferences) or whether one or many non-dominated solutions are obtained in one run.

Weighted, ε-constraint and goal programming methods require a priori preference of the decision maker, and find one non-dominated solution in one run. By changing the preference, one can find more non-dominated solutions but this requires more than one run. Many of these were proposed before 1990, and so can be considered as classical methods. They generally transform a MOO problem into a single-objective optimization problem, which can then be solved by a suitable deterministic or stochastic method. Methods with posteriori or without articulation of preferences can find many non-dominated solutions in one run. These have been developed after 1990 and can be termed "modern methods." Many of them use stochastic global optimization methods such as genetic algorithms, differential evolution and particle swarm optimization. There are also interactive methods, which incorporate the decision-maker's preference during the search for non-dominated solutions. A comprehensive review of MOO methods can be found in Miettinen (1999), Coello Coello *et al.* (2002) and Marler and Arora (2009).

The available MOO methods have their own strengths and weaknesses for solving application problems, and it is important to identify and understand them for two reasons: one is to choose and use the appropriate method for the application on hand and another is for developing new and more robust MOO techniques. In particular, the study and development of stochastic methods has been an active research area in MOO since the early 1990s because these strategies can find multiple non-dominated solutions in a single run. These methods do not require any assumptions on the objective functions and their mathematical characteristics. Stochastic MOO methods include adaptations of simulated annealing, genetic algorithms, evolutionary approaches, tabu search, differential evolution and particle swarm optimization for multiple objectives. One stochastic MOO solver, namely, elitist nondominant sorting genetic algorithm (NSGA-II) has been used for solving many chemical engineering application problems (see Chapter 3) because of its ready availability and effectiveness. The convergence performance of classical MOO methods depends on the shape and continuity of the Pareto-optimal front. Stochastic MOO methods are less sensitive to the characteristics of the optimization problem (e.g., type of objective functions, decision variables and constraints) and the Pareto-optimal front.

The performance of MOO methods can be quantified using different metrics based on computational requirement (such as CPU time and number of function evaluations), the closeness of the obtained non-dominated solutions to the true/exact Pareto-optimal front (known only for benchmark problems) and the spread of the non-dominated solutions found.

Table 1.1 *Summary of relevant journal articles on MOO of chemical engineering applications.*

Period	Number of journal papers	Major application areas of MOO	Reference
Before the year 2000	≈ 30	Process design and control, chemical reaction engineering, biochemical engineering, waste treatment and pollution control, electrochemical process	Bhaskar *et al.* (2000)
From 2000 to mid-2007	≈ 100	Process design and operation, petroleum refining and petrochemicals, biotechnology and food technology, pharmaceuticals, polymerization	Masuduzzaman and Rangaiah (2009)
From 2007 to mid-2012	≈ 230	Process design and operation, petroleum refining, petrochemicals, polymerization, power generation, pollution control, renewable energy, hydrogen production, fuel cells	Chapter 3 of this book

Analysis of MOO results has been mainly focused on the values of objective functions (i.e., in the objective function space shown in Figure 1.1). It is equally important to review and understand the trends of values of decision variables corresponding to the non-dominated solutions as one of these has to be selected and implemented to achieve the desired tradeoff solution for the application under study.

1.3 Multi-Objective Optimization in Chemical Engineering

In chemical engineering, the presence of several conflicting objectives to be optimized simultaneously is a common situation and, consequently, MOO applications have grown considerably since the late 1990s. In fact, the importance of this optimization approach is reflected by a significant increase in the number of papers published in different journals—see Table 1.1. Recent chemical engineering applications of MOO are summarized in Chapter 3 of this book. This rapidly growing interest in the chemical engineering community has prompted the development of new MOO methods, concepts and novel process applications.

Reported MOO of chemical engineering applications include scheduling, production planning and management of chemical processes, process design and simulation of unit operations (e.g., crystallization and distillation), chemical reaction engineering, pollution prevention and control, industrial waste management, water recycling and wastewater minimization, supply chain with environmental considerations, biorefinery process design and integration (Bhaskar *et al.*, 2000; Masuduzzaman and Rangaih, 2009). In particular, novel chemical engineering applications combine economic objectives with process performance metrics (such as conversion and energy consumption) and also environmental objectives

obtained, for example, from life-cycle analysis. These applications include new emerging areas such as the design of renewable energy systems and the distributed energy resources planning (see Chapter 3). As stated by Garcia *et al.* (2012), the inclusion of environmental concerns as optimization targets for process design in chemical engineering and other fields has increased the application and uses of MOO tools.

In summary, MOO is playing an important role in chemical engineering, and a variety of MOO techniques can be used for chemical engineering applications. There is no doubt that the number and type of MOO of chemical engineering applications will increase in the coming years. In fact, many chemical engineering problems that consider only one objective can be reformulated as MOO problems to develop a more realistic approach to their solution. Thus, MOO can be used to quantify and understand the tradeoffs among the conflicting objectives in the optimization of a chemical process.

1.4 Scope and Organization of the Book

This book is organized in three parts. Part I consists of Chapters 1 to 3 and provide an overview to MOO and its chemical engineering applications. Chapters 4 to 8, in Part II, cover developments in MOO; although these are contributed by chemical engineering researchers, they are applicable to and useful in other disciplines too. The focus of Chapters 9 to 17, in Part III, are on MOO applications in chemical engineering. Chapters 2 to 17 are briefly summarized in the following paragraphs.

Chapter 2 addresses the optimization of pooling problems for two objectives using the ε-constraint method, contributed by Zhang and Rangaiah. It describes pooling problems, presents a new formulation and illustrates the application of the ε-constraint method for two objectives. Pooling problems are optimization problems of importance in petroleum refineries. They are likely to have multiple minima, and so a global optimization method is required to find the optimal solution. The solution of pooling problems for single objective has been studied using many deterministic global optimization algorithms. However, there has been no attempt to solve the pooling problems for multiple objectives. Hence, in this chapter, pooling problems are optimized for two objectives using the ε-constraint method along with a recent stochastic global optimization algorithm, namely, integrated differential evolution (IDE). Further, a new formulation that does not involve equality constraints is described and used. Many pooling problems from the literature are optimized for two objectives, and the results demonstrate the potential of MOO for finding tradeoff solutions for pooling problems. In short, this chapter illustrates the application of a popular classical method, namely, ε-constraint method to the optimization of pooling problems.

Multi-objective optimization has found numerous applications in chemical engineering, particularly since the late 1990s. Earlier, Bhaskar *et al.* (2000) have reviewed applications of MOO in chemical engineering. Masuduzzaman and Rangaiah (2009) have reviewed reported applications of MOO in chemical engineering from the year 2000 until middle of 2007. In Chapter 3, Sharma and Rangaiah summarize about 230 articles on MOO in chemical engineering and related areas, published from the year 2007 until June 2012, under six groups: (1) process design and operation, (2) petroleum refining, petrochemicals and polymerization, (3) food industry, biotechnology and pharmaceuticals, (4) power generation and carbon dioxide emissions, (5) renewable energy, and (6) hydrogen production and fuel

cells. The first group and the last three groups have seen significant increase in the number of papers published since 2007.

Part II on MOO developments begins with Chapter 4, where Sharma, Nabavi and Rangaiah analyze the performance of jumping gene adaptations of elitist non-dominated sorting genetic algorithm (NSGA-II), which has been used to optimize many process design and operation problems for two or more objectives. In order to improve the performance of this algorithm, jumping gene concept from natural genetics has been incorporated in NSGA-II. Several jumping-gene adaptations have been proposed and used to solve mathematical and application problems in different studies. In Chapter 4, four jumping-gene adaptations are selected and comprehensively evaluated on a number of bi-objective unconstrained and constrained test functions. Three quality metrics, namely, generational distance, spread and inverse generational distance are employed to evaluate the distribution and convergence of the obtained Pareto-optimal solutions at selected intermediate generations and the final generation. Additionally, a search termination criterion based on the improvement in the Pareto-optimal front, has been described and used to check convergence of NGSA-II with the selected jumping-gene adaptations.

In Chapter 5, Sharma and Rangaiah discuss an improved constraint handling technique for MOO and its application to two fermentation processes. Constraints besides bounds are often present in MOO problems in chemical engineering; these arise from mass and energy balances, equipment limitations, and operation requirements. Penalty function and feasibility approaches are the popular constraint handling techniques for solving constrained MOO problems by stochastic global optimization (SGO) techniques, such as genetic algorithms and differential evolution. This chapter briefly reviews selected applications of these constraint-handling approaches in chemical engineering. In the penalty-function approach, solutions are penalized based on constraint violations; its performance depends on the penalty factor, which necessitates selection of a suitable value for the penalty factor for different problems. Generally, the feasibility approach is good for solving problems with inequality constraints due to their large feasible regions. It gives higher priority to a feasible solution over an infeasible solution, but this limits the diversity of the search. Feasible search space is extremely small for equality-constrained problems and so the feasibility approach may not be effective for handling equality constraints. The approach of adaptive relaxation of constraints in conjunction with feasibility approach, addresses this issue by relaxing feasible search space dynamically. This approach has been found to be better and effective for solving SOO problems with equality and inequality constraints by SGO techniques. In Chapter 5, a modified adaptive relaxation with feasibility approach is explored for solving constrained MOO problems by stochastic optimizers, and its performance is compared with that of feasibility approach alone. For this, the modified adaptive relaxation with feasibility approach is incorporated in the multi-objective differential evolution (MODE) algorithm and tested on two benchmark functions with equality constraints. Finally, MODE with the proposed constraint handling approach is applied to optimize two fermentation processes for multiple objectives.

A robust multi-objective genetic algorithm (RMOGA) with online approximation under interval uncertainty is the subject of Chapter 6 by Hu, Butt, Almansoori, Azarm and Elkamel. Optimization of chemical processes is usually multi-objective, constrained and has uncertainty in the process inputs, variables and/or parameters. This uncertainty can produce undesirable variations in the objective and/or constraints. The traditional

multi-objective genetic algorithm (MOGA) assumes that all inputs are deterministic. However, optimal solutions obtained by it can be sensitive to input uncertainty and degrade the solutions. The goal in RMOGA is to obtain solutions that are optimum while also being relatively insensitive to uncertainty. For this, one nested approach and another sequential approach are presented in Chapter 6. In both of them, a measure of robustness is considered using a worst-case analysis, which assumes that the uncertainty in inputs is expressed by an interval with known lower and upper bounds. In the nested approach, an upper level problem identifies and improves candidate solutions, while a lower level subproblem evaluates their robustness. In the sequential approach, the MOO problem is first solved to obtain optimal solutions, and then the robustness of each optimal solution is evaluated. Both nested and sequential RMOGA can be computationally costly. To ease the computational cost, an online approximation-assisted method is used in both approaches. The purpose of the approximation is to replace the computationally intensive evaluation of objectives and constraints with a surrogate model (which is computationally much less intensive) while adaptively improving the accuracy of the approximation as the search progresses. One numerical example and a petroleum refinery example are used to demonstrate and compare the applicability of the two RMOGA approaches.

Another technique to handle uncertainty in nonlinear process models is presented in Chapter 7 by Mitra. Among the various preventive uncertainty handling techniques, the chance-constrained programming (CCP) has gained considerable interest in recent times due to certain advantages of its usage over its competitors. The CCP is different from deterministic optimization since the former has a stochastic component attached to it. The complexity involved in propagating the uncertainties in stochastic parameters to the corresponding constraints and objective functions of the deterministic equivalent optimization formulation is one of the key challenges in CCP. In Chapter 7, various facets of CCP has been presented and explained through examples of different types. Problem formulation using CCP under different scenarios has been discussed and demonstrated with examples from the literature and the real world. It has been also shown how stochastic component present in the CCP formulation leads to solution reliability which has an inverse relationship with solution quality.

Chapter 8, the last in Part II, is on fuzzy MOO for metabolic reaction networks by mixed-integer hybrid differential evolution (MIHDE) by Wang and Wu. In the optimization of metabolic reaction networks, designers have to manage the nature of uncertainty resulting from qualitative characters of metabolic reactions, for example the possibility of enzyme effects. A deterministic approach does not give adequate representation of metabolic reaction networks with uncertain characters. Fuzzy optimization formulations can be applied to cope with this problem. Chapter 8 introduces a generalized fuzzy MOO problem (GFMOOP) for finding the optimal engineering interventions on metabolic network systems considering the resilience phenomenon and cell viability constraints. This approach first formulates a constrained MOO problem that considers the resilience effects and minimum set of manipulated enzymes simultaneously by combining the concepts of minimization of metabolic adjustment (MOMA) and regulatory on/off minimization (ROOM). In addition, the nonlinear kinetic equations were included in the optimization formulation, and so it was formulated as a constrained mixed-integer nonlinear programming (MINLP) problem. Mixed-integer hybrid differential evolution (MIHDE) was extended to solve constrained MINLP problems through the implementation of constraint

handling techniques. The fuzzy goal attainment approach implemented in MIHDE was used to solve GFMOOPs for the identification of optimal genetic manipulation strategies on metabolic reaction networks, and its effectiveness is discussed in Chapter 8.

Chemical engineering applications of MOO, in Part III, begin with Chapter 9 by Punnapala, Vargas and Elkamel, on parameter estimation in phase-equilibrium modeling. Phase-equilibrium calculations play a vital role in the design, development, operation, optimization and control of chemical processes. Equations of state or activity coefficient models are normally tuned to match certain properties in order to give an accurate description of the phase behavior. This chapter introduces the application of MOO for parameter estimation wherein a model is simultaneously fit to two or more conflicting properties. As an example, the parameters of NRTL activity coefficient model are estimated by fitting the parameters to vapor-liquid equilibrium data and heat of mixing (excess enthalpy). Particle swarm optimization is used for this MOO.

Chapter 10 by Bonilla-Petriciolet, Sharma and Rangaiah considers another application of MOO to phase equilibrium data modeling. In this chapter, MOO is applied for simultaneous parameter estimation and data reconciliation of vapor-liquid equilibrium using the error-in-variable formulation and activity coefficient models. Multi-objective differential evolution with a tabu list is used for obtaining the Pareto-optimal front of data reconciliation problems with three and four objectives. The application of some criteria of interest in thermodynamic modeling is illustrated to characterize the solutions obtained from the Pareto-optimal fronts of reconciled phase equilibrium data. The results show that MOO is an alternative and reliable approach for performing data reconciliation in phase equilibrium modeling.

Al-Mayyahi, Hoadley and Rangaiah describe multi-objective process synthesis with embedded energy integration in Chapter 11. Energy integration decreases energy costs of industrial processes by increasing heat recovery and reducing utilities consumption. Several potential opportunities for improving the energy efficiency and, consequently, reducing CO_2 emissions of petroleum refining processes have been investigated over the years via implementing heat integration within a single process unit or among different refining processes. However, the tradeoff between CO_2 emissions and other economic or operating objectives has not been widely covered. In Chapter 11, MOO has been implemented *for* an integrated model of a crude distillation (CDU) and fluidized catalytic cracking (FCC) complex using a binary-coded NSGA-II to investigate the tradeoff between CO_2 emissions and economic objectives. The CDU includes the atmospheric distillation unit (ADU), the vacuum distillation unit (VDU) and the crude preheat train, whilst the FCC model includes the reactor/regenerator section, the feed preheat train, the main fractionator and flue gas heat and power recovery sections. Pinch analysis is used to maximize the heat recovery within the integrated model and evaluate the distribution of utilities related to emissions. The Pareto-optimal results including optimal operating conditions are presented and their significant features are discussed.

In Chapter 12, Azzaro-Pantel and Pibouleau describe ecodesign of chemical processes with MOGAs. Process synthesis is a complex activity involving many decision makers and multiple levels of decision steps. From these many alternatives, the designers want to select the one that best suits both economic and environmental criteria. This chapter shows that MOO and multiple choice decision making (MCDM) techniques can be useful for the ecodesign of a process. Two examples illustrate the determination of eco-friendly and cost-effective designs: the so-called Williams and Otto process and the well-known

benchmark process for hydrodealkylation (HDA) of toluene to produce benzene. This chapter deals with the definition of various objectives for designing eco-efficient processes, by considering simultaneously ecological and economic features. An improved variant of NSGA-II is implemented for solving the resulting MOO problems. The environmental burdens are evaluated by means of a decision support tool dedicated to the management of plant utilities and to the emission control of pollutants. After finding the Pareto-optimal solutions, a MCDM technique is used to discover the most interesting tradeoff design alternatives.

Tarafder presents modeling and MOO of a chromatographic system in Chapter 13. Chromatography is a separation technique, which plays a crucial role in the downstream of several pharmaceutical and fine chemical industries. The chromatographic units in these industries handle gram to kilogram scale of very high-value products per day, and they may be required to be redesigned after a period of time, depending on the changes in the product lines or other requirements. The current industrial practice mostly relies on empirical methods to develop the operating conditions; but, given the high cost of products, there is a huge incentive of applying model-based MOO studies in improving the performance of such processes. Chapter 13 describes the development of a model-based optimization program, and then demonstrates the ways of conducting optimization studies with this model. The example chosen for this chapter is the separation of enantiomers in batch processes. In the industries, there is a strong requirement for faster separation of enantiomers, but that has to sacrifice the product recovery as the sample mixture may not get enough time to separate entirely. But, as recovery is a critically important parameter for process economics, the situation leads to an optimization problem having conflicting objectives. Chapter 13 provides the basic understanding of developing a mathematical model to simulate such a system, formulate the objective functions, identify the constraints and the most useful decision variables, and finally, with the help of a genetic algorithm, determine the Pareto-optimal solutions.

Estimation of crystal size distribution by image thresholding based on MOO is the subject of Chapter 14 by Periasamy and Lakshminarayanan. Crystallization process can be effectively controlled by monitoring the crystal size distribution (CSD), which can be estimated using particle vision and measurement (PVM) images. Image segmentation based on thresholding is critical in this regard. Generally, the threshold is selected by optimizing a single objective. Based on the type of thresholding used, segmentation can be improved. Hence, in this work, optimum threshold is calculated by solving a MOO problem. The two objectives used are within-class variance and overall probability of error. This MOO problem is solved based on the plain aggregating approach and simulated annealing by assigning appropriate weights to each objective function. The MOO-based thresholding overcomes the limitations and outperforms the thresholding performed by either of the single objectives. The segmented images are further processed by means of feature extraction to estimate the CSD. The algorithm was tested on a set of artificially generated crystallization images, and its accuracy was calculated by comparing the CSD estimated to the data used to generate the artificial images. This accuracy was found to be around 90% for images in which about 20–25 particles exist.

In Chapter 15 by Gudena, Rangaiah and Lakshminarayanan, a hybrid steam-stripper membrane process for continuous bioethanol purification is optimized for multiple objectives. Several ethanol-water separation technologies for continuous recovery and

purification of bioethanol from fermentation broth are discussed in the literature. Recently, a hybrid steam-stripping membrane-separation process is proposed and shown to reduce energy consumption for separation by nearly half when compared to the conventional distillation process. This chapter discusses detailed modeling of the hybrid stripper-membrane separation process in Aspen-Plus™ followed by its MOO using the ε-constraint method. Important objectives, namely operating cost per unit of ethanol produced, ethanol purity (as there is no consensus on the limit for water in bioethanol as a fuel in different countries) and ethanol loss in the waste stream, are considered. Pareto-optimal solutions obtained for these conflicting objectives are presented and discussed.

The design of the cumene process for economic, environmental and safety (EES) objectives is described in Chapter 16 by Sharma, Lim and Rangaiah. Safety is very important in the process industry, but it has received much less attention than economic objectives in process optimization. Although it is difficult to quantify process safety at the preliminary design stage, several safety indices have been proposed to assess inherent safety of chemical processes. In this chapter, these safety indices are reviewed, and one of them is chosen for MOO of the cumene process design. Integrated inherent safety index (I2SI), material loss from the cumene process and total capital cost, respectively, are used as safety, environmental and economic objectives for MOO. Three bi-objective and one tri-objective optimization problems for the cumene process are solved using NSGA-II. The non-dominated solutions obtained are presented and discussed. These are useful for better understanding of tradeoffs among the EES objectives and for selecting a suitable design of cumene process.

In the last chapter of Part III and also the book (Chapter 17), Vandervoort, Thibault and Gupta develop new proportional-integral (PI) controller tuning methods for processes represented by a first-order plus dead time transfer function. The developed methods involve approximating the Pareto-optimal domain associated with the minimization of three performance criteria: the integral of the time-weighted absolute error, the integral of the squares of the differences in the manipulated variable, and the settling time. Two tuning methods were developed, achieving optimal controller performance by specifying either one of the controller input parameters or the desired values of the performance criteria. The developed controller tuning methods were compared to several previously developed controller correlations. Finally, the developed tuning methods were applied to a fourth-order process subjected to a set point change and a disturbance, and shown to provide excellent performance.

In summary, chemical engineers working in industry will find the introductory chapters in Part I and the application chapters in Part III beneficial when using MOO in applications related to their jobs. Methodological developments in MOO covered in part II will be of particular interest to researchers from diverse fields who are interested in MOO. Chemical engineering students, particularly those learning or pursuing research in optimization including MOO, will find all chapters in this book useful in their studies. Many chapters in this book have exercises at the end, and some chapters provide useful programs / files on the book web site. Depending on their background and interest, readers can choose to read the entire book, one or more parts, or particular chapters.

Increasing importance and significance of MOO in chemical engineering studies and practice can be seen from the article by Garica *et al.* (2012) on teaching mathematical modeling software for MOO in chemical engineering courses, and the article by Lee *et al.*

(2008) on optimizing process plants for more than one objective. Availability of Excel-based MOO programs (e.g., Sharma *et al.*, 2012) will further facilitate MOO of more applications in chemical engineering. We hope the book in your hand will help to increase the use of MOO in both academia and industrial practice. We also anticipate the availability of selected modern methods of MOO for generating Pareto-optimal fronts for chemical engineering applications, in commercial process simulators such as Aspen Plus and Aspen Hysys in the coming years.

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