Chapter 1
Introduction

The fundamental concepts used in this book are described below. To implement the link between any process simulator and metaheuristic techniques, the methodology has been divided in three parts: simulation, optimization, and link software; and the involved concepts are described as follows.

1.1 Process Simulation

A mathematical model of a chemical process is a simplified representation of the physicochemical behavior of a real process, which is used to predict values of output variables for given input variables and process design (including operating) variables. A model can be used for what-if studies and process troubleshooting, and it has many applications for process optimization, process control, and operator training. Models are often difficult to solve analytically, and so they are mostly solved numerically (Sharma and Rangaiah 2016).

Process simulation allows predicting the behavior of a process by using basic engineering relationships, such as mass and energy balances, and phase and chemical equilibrium. Given reliable thermodynamic data, realistic operating conditions, and rigorous equipment models, one can simulate the plant behavior. Process simulation enables to run many cases, conduct "what-if" analyses, and perform sensitivity studies and optimization runs. With simulation, one can design better plants and increase profitability in existing plants. Process simulation is useful throughout the entire life cycle of a process, from research and development through process design to production (AspenTech 2015).

Modeling refers to all the steps involved in developing and validating a model for the process, whereas simulation refers to the use of the developed model for studying the process behavior/response for one or more sets of input and design variables. In general, modeling and simulation are used to optimize the process

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operation and design. Optimization improves the performance of a process by changing the operating conditions such as temperature, pressure, and flow rate of process streams but without changing the size of any equipment or process flowsheet. Process retrofitting and revamping refer to redesign a plant for specific objective(s), such as increasing throughput, decreasing energy consumption, and revising product quality. This is achieved by changes in existing equipment and/or addition of new equipment (leading to a new process configuration) besides changes in operating conditions (Sharma and Rangaiah 2016).

1.2 Searching Methods

Optimization is the act of making something as good as possible (Cambridge dictionary). The word optimum means "the best." Optimization consists in finding the optimum point in which the best values are found for certain variables and in which they achieve some specific objectives. There are different search methods to achieve optimization, which will be analyzed in depth in the corresponding chapter.

The decision variables correspond to those that have been previously determined and will be manipulated in order to find the optimal point. These variables must operate within a range in which they offer feasible results for the objectives being sought; this is the operating range. Also, the decision variables can be subject to certain constraints that the user must know for the studied processes; these constraints help to limit the search range and make the optimization more efficient, reducing the computation time.

The objective function is an equation in which is reflected the performance of the process that is being optimized; it is achieving its maximum or its minimum value by manipulating the variables of dissolution and considering the established search restrictions.

1.2.1 Classification of Search Methods

General search and optimization techniques are classified into three categories: enumerative, deterministic, and stochastic (Coello-Coello et al. 2002). Figure 1.1 shows common examples of each type. Some authors classify calculus-based methods in indirect and direct, and classify evolutionary computation in evolution strategies, evolutionary programming, genetic algorithms, and genetic programing (Devillers 1996).

To overcome some drawbacks associated to the deterministic optimization approaches, metaheuristic optimization approaches have been reported (Wang and Tang 2013; Guo et al. 2014; Ouyang et al. 2015; Wong et al. 2016). The metaheuristic optimization approaches mimic some evolution processes and are based on

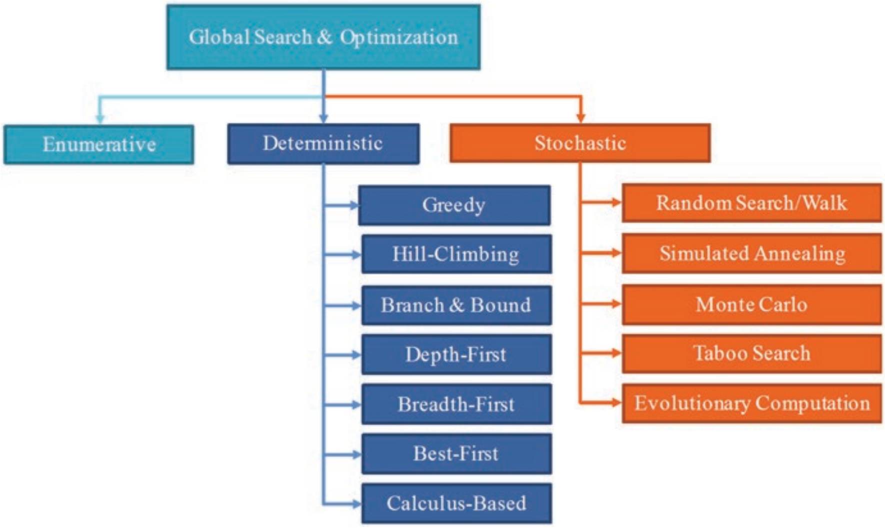

Fig. 1.1 Global optimization approaches and different classes of search methods (Coello-Coello et al. 2002; Devillers 1996)

repeatedly simulating a given process to assign a fitness function for given values of the degrees of freedom (Sharma and Rangaiah 2016). This way, the possibility to get trapped prematurely in a suboptimal solution is avoided (Devillers 1996), the complication associated to the form of the optimization model is avoided (Sharma and Rangaiah 2014), and mainly because these are based on simulation of the process, these can be easily linked to the process simulators to optimize different flowsheets.

1.2.2 Deterministic Algorithms

Deterministic methods have been successfully used in solving a wide variety of problems. However, these methods are inefficient for solving non-convex and nonlinear problems. For the implementation of these optimization methods, it is necessary to implement all the equations that describe the behavior of the process by the formulation of a mathematical model.

Deterministic methods are often ineffective when applied to NP-complete or other high-dimensional problems because they are limited by their requirements associated to the problem domain, knowledge (heuristics), and the search space, which can be exceptionally large. Because many real-world scientific and engineering multi-objective problems (MOPs) exhibit one or more of the abovementioned characteristics, stochastic searches have been developed as alternative approaches for solving these irregular problems (Coello-Coello et al. 2002).

1.3 Interaction Between Programs

When the word link is mentioned in this book, it refers to the relationship between programs for the purpose of controlling or sending and receiving data obtained in different software. The link between programs can be established through the use of internal tools of some of the programs or through the instructions of a third program.

Visual Basic for Applications (VBA) is the language of the Microsoft (MS) operating system (Windows) that is used for program applications. Many of the programs and add-ons that are used in Windows are developed in this language, so there are common elements that can be manipulated through this platform.

Microsoft COM (Component Object Model) technology in the Microsoft Windows-family of operating systems that enables software components to communicate (microsoft.com), for this reason, this technology is used to achieve the link between the simulation software and the program in which the optimization algorithm is based. The details of the use of the COM technology will be described in the corresponding chapter.

1.4 Nomenclature

ACM Aspen Custom Modeler
COM Component Object Module
MOP Multi-objective problems
MS Microsoft®
VBA Visual Basic for Application