Chapter 16

Multi-Objective Optimization Programs and their Application to Amine Absorption Process Design for Natural Gas Sweetening

Shivom Sharma[1], Gade Pandu Rangaiah[2]*, François Maréchal[1]

1 - Industrial Process and Energy Systems Engineering
Ecole Polytechnique Fédérale de Lausanne, Sion, Switzerland
2 - Department of Chemical & Biomolecular Engineering
National University of Singapore, Singapore 117585

* Corresponding author: gprangaiah@gmail.com

Abstract

This chapter presents three MS Excel programs, namely, EMOO (Excel based Multi-Objective Optimization), NDS (Non-Dominated Sorting) and PM (Performance Metrics) useful for Multi-Objective Optimization (MOO) studies. The EMOO program is for finding non-dominated solutions of a given MOO problem. It has both binary-coded and real-coded NSGA-II (Elitist Non-Dominated Sorting Genetic Algorithm), and two termination criteria based on chi-squared test and steady state detection. The known/true Pareto-optimal front for the application problems is not available unlike that for benchmark problems. Hence, a procedure for obtaining known/true Pareto-optimal front is described in this chapter. The NDS program is for non-dominated sorting and crowding distance calculations of the non-dominated solutions obtained from several optimization runs using same or different MOO programs. The PM program can be used to calculate the values of performance metrics between the non-dominated solutions obtained using a MOO program and the true/known Pareto optimal front. It is useful for comparing the performance of MOO programs to find the non-dominated

solutions. Finally, use of EMOO, NDS and PM programs is demonstrated on MOO of amine absorption process for natural gas sweetening.

Keywords: Multi-Objective Optimization, NSGA-II, Binary Coding, Real Coding, Performance Metrics, Termination Criteria, Non-Dominated Sorting, Crowding Distance Calculations, Amine Absorption Process, Natural Gas Sweetening.

16.1.   Introduction

In recent times, optimization has been widely used in engineering, science, economics, business and other areas. In the process industries, plant performance is analyzed and/or optimized for several conflicting objectives such as capital cost, operating cost, energy consumption, environmental impact and safety. Many people including engineering practitioners and students are familiar with MS Excel, and they use it for data analysis and numerous calculations. In fact, MS Excel dominates as the engineers' tool of choice due to its familiarity and ready availability compared to other programs/platforms (e.g., MATLAB and FORTRAN).

In this chapter, three MS Excel programs useful for Multi-Objective Optimization (MOO) are presented:

- In Section 16.2, EMOO: a program for generating the non-dominated solutions (also known as Pareto-optimal front) of a MOO problem is described;
- In Section 16.7, NDS: a program for non-dominated sorting and crowding distance calculations of non-dominated (i.e., optimal) solutions obtained from one or more optimization runs is discussed;
- In Section 16.8, PM: a program for calculating the performance metrics between the obtained non-dominated solutions and the known/true Pareto-optimal front is presented.

To illustrate the application of the EMOO, NDS and PM programs, the Amine Absorption Process (AAP) for acid gases removal from natural gas is considered. The process flowsheet is simulated in Aspen HYSYS and then optimized using the EMOO program for two objectives: capital cost and annual operating cost. For this, the EMOO program is interfaced

with Aspen HYSYS via Visual Basic for Applications (Sharma and Rangaiah, 2016).

Genetic Algorithms (GA), developed for Single Objective Optimization (SOO), mimic the natural genetic processes of crossover, mutation and selection. Based on it, Elitist Non-Dominated Sorting Genetic Algorithm (NSGA-II) was developed for MOO (Deb *et al*., 2002). Sharma *et al*. (2012) created an MS Excel-based MOO (EMOO) program, which employs binary-coded NSGA-II and Maximum Number of Generations (MNG) as the termination criterion. In this program, probably the first of its type for MOO, MS Excel worksheets are used as the program interface, specifying algorithm parameters values, the calculation of objective functions and constraints, and the display of results. Visual Basic for Applications (VBA) is used for implementation of the binary-coded NSGA-II. The EMOO program can be used to find the non-dominated solutions of a MOO problem.

Generally, MNG is used as the termination criterion for stochastic MOO algorithms. It must be sufficiently large to ensure convergence (or closeness) to the global optimum, and so this can lead to unnecessary generations without much improvement in the solution quality. It is worth considering other termination criteria that can terminate the search at the right time and save the computation time. Trautmann *et al*. (2009) developed a convergence detection method, based on statistical tests on performance metrics, which can be used as a termination criterion for stochastic MOO algorithms. Sharma and Rangaiah (2013a) included chi-squared test based termination criterion in multi-objective differential evolution program. Rhinehart (2014) developed a convergence criterion for SOO based on steady-state detection by comparing the objective function variance estimated by two different ways. Recently, Wong *et al*. (2016) included real-coded NSGA-II, chi-squared test based termination criterion and the novel steady-state detection termination criterion in the EMOO program. These two termination criteria have shown good performance on several test and application problems (Sharma and Rangaiah, 2013a; Sharma and Rangaiah, 2014; Wong *et al*., 2016).

In MOO, performance metrics are used to characterize the quality of the obtained non-dominated solutions using a given method/program, and to compare performance of different algorithms quantitatively. Some

of them are used to check the convergence of the non-dominated solutions to the known/true Pareto-optimal front (i.e., closeness of the two fronts) while some others are used to check the spread of the non-dominated solutions obtained. Some other performance metrics can be used to evaluate both convergence and spread of the non-dominated solutions obtained (Deb, 2001). In this chapter, four important performance metrics are described, and also PM program in MS Excel for calculating them is presented.

Pareto-optimal solutions (i.e., true/known non-dominated solutions) for real world application problems are not known in advance, and yet calculation of performance metrics requires them. Hence, the application problem is solved many times using a sufficiently large MNG. The optimization results from different runs are consolidated and sorted to find the known/true Pareto-optimal front, which is then used for calculating the performance metrics. In this chapter, NDS program in MS Excel is developed to find the non-dominated solutions among the optimal solutions obtained in different runs. Then, these non-dominated solutions can be used as the known/true Pareto-optimal front for performance metric calculations.

16.2.   EMOO Program

Several multi-objective genetic algorithms have been presented in the literature (e.g., Deb, 2001; Coello Coello *et al*., 2007). They belong to the class of Pareto generating techniques, as they can generate the Pareto-optimal front in a single run. Genetic algorithms are search methods, mimicking the natural selection process, for global optimization. One implementation of genetic algorithms for MOO is NSGA proposed by Srinivas and Deb (1995). Later, Deb *et al*. (2002) improved NSGA by introducing elitism and diversity into NSGA-II. Two other major improvements in NSGA-II are fast non-dominated sorting of population based on Pareto dominance and the crowding distance assignment for calculating the density measure (Deb *et al*., 2002).

NSGA-II has found many applications in Chemical Engineering (Chapter 2 in this book; Cheah and Rangaiah, 2009; Sharma and

Rangaiah, 2013b; Rangaiah *et al*., 2015), and so it was chosen for the development of an Excel based MOO (EMOO) program. Both binary- and real-coded NSGA-II with two termination criteria are implemented in this program. The algorithm used in the EMOO program is briefly described below, and its flow-chart is given in Fig. 16.1. Interested readers are referred to Deb *et al*. (2002) for details on population generation, selection, crossover, mutation and other calculations.

1. Generate the initial/parent population of NP individuals inside the bounds on decision variables, using uniformly distributed random numbers between 0 and 1. Compute values of objective functions and constraints for all individuals in the initial population.

2. The parent/current population of NP individuals participates in the selection, crossover and mutation operations of genetic algorithms, to generate new NP individuals (child population). Calculate values of objective functions and constraints for the child population.

3. Combine the child population with the parent/current population to produce the combined population of 2NP individuals.

4. Find the number of individuals dominating each individual in the combined population. NSGA-II handles inequality constraints by constrained-dominance criteria, also known as feasibility (first) approach (Deb *et al*., 2002). According to this, individual A is dominating individual B if any of the following conditions is true.

   • Both the individuals are feasible, and individual A is dominating individual B if individual A is better than individual B in at least one objective and equal to individual B in other objectives. Note that individuals A and B are non-dominated to each other if A is better than B in at least one objective and B is better than A in at least one other objective.

   • Individual A is feasible, and individual B is infeasible.

   • Both the individuals are infeasible, but individual A has a smaller number of violated constraints compared to individual B. If both individuals have the same number of violated constraints, then individual A has lesser total absolute constraint violation than individual B.

5. The number of individuals (nd) dominating each individual in the combined population is calculated. First rank is assigned to non-

dominated individuals with nd = 0 (i.e., they are not dominated by any other individual). Then, first rank individuals are excluded from the combined population, and non-dominated individuals (nd = 0) in the remaining population are assigned second rank. This ranking procedure is repeated until all individuals in the combined population are ranked.

6. Sort all the individuals in the combined population according to their Pareto ranks found in the previous step, and then find the Pareto rank of NP[th] individual. This rank is denoted as the ndc.

7. For all the individuals with Pareto rank = ndc, calculate the crowding distance in the objective function space.

8. Sort all the individuals according to their Pareto rank, and then sort the individuals with Pareto rank = ndc in the order of decreasing crowding distance. The first NP individuals will form the current population in the next generation.

9. Repeat steps 2 to 8 for the specified MNG or until the specified termination criterion is satisfied.

The EMOO program cannot solve equality constraints in the optimization problem. If the MOO problem has equality constraints, they have to be solved as part of objectives and inequality constraints. Some equality constraints can be eliminated before optimization, as they can be solved for suitable decision variables thus reducing the problem size. However, it may not always be possible to eliminate all equality constraints before optimization.

Both binary- and real-coding of decision variables for NSGA-II are implemented in the EMOO program. In the binary coding, individuals (i.e., values of their decision variables) are represented by binary strings, whereas they are represented by real numbers in the real coding. In the binary-coded NSGA-II, binary tournament selection for participation in crossover and mutation operations, crossover by single point, two-point and uniform schemes, and bit-wise mutation are employed (in Step 2 of the algorithm given above). The same Step 2 of real-coded NSGA-II uses binary tournament selection for participation in crossover and mutation operations, simulated binary crossover and non-uniform mutation.

```
┌─────────┐      ┌──────────────────────────────────────────────┐
│  Start  │─────▶│ Set values of NP, MNG, pc, pm, ηc, b_num.    │
└─────────┘      └──────────────────────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Randomly initialize population, and evaluate values of │
        │ objective functions and constraints for all the        │
        │ individuals in the population (call process simulator,  │
        │ if necessary) (Step 1).                                │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
                  ┌──────────────────────────────┐
                  │ Set generation number, G = 1. │
                  └──────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Select NP individuals from the current population by   │
        │ binary tournament, and store them in the mating pool   │
        │ (Step 2).                                              │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
                  ┌──────────────────────────────┐
                  │ Set individual number, i = 1. │
                  └──────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Randomly select two individuals from the mating pool.  │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Generate two new individuals by crossover (Step 2).    │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Mutation on newly generated individuals (Step 2).      │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Check violation of decision variable bounds;           │
        │ if there is a violation, randomly re-initialize        │
        │ that decision variable inside the bounds.              │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Store new individuals in the child population.         │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
              Yes        ◇ Is i < NP/2? ◇
  ┌───────────┐◀─────────         │ No
  │ i = i + 1 │                   ▼
  └───────────┘
        ┌──────────────────────────────────────────────────────┐
        │ Evaluate values of objective functions and constraints │
        │ for new NP Individuals (call process simulator,         │
        │ if necessary).                                         │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Combine new NP individuals (child population)          │
        │ with current/parent population (Step 3).              │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Rank 2NP individuals using constrained dominance       │
        │ criteria, and calculate crowding distance if required  │
        │ (Steps 4-7).                                           │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
        ┌──────────────────────────────────────────────────────┐
        │ Select NP individuals for the next generation          │
        │ as discussed in the Text (Step 8).                    │
        └──────────────────────────────────────────────────────┘
                                    │
                                    ▼
              No       ◇ Is termination       ◇  Yes   ┌──────┐
  ┌───────────┐◀───────  criterion satisfied?  ───────▶│ Stop │
  │ G = G + 1 │                                         └──────┘
  └───────────┘
```
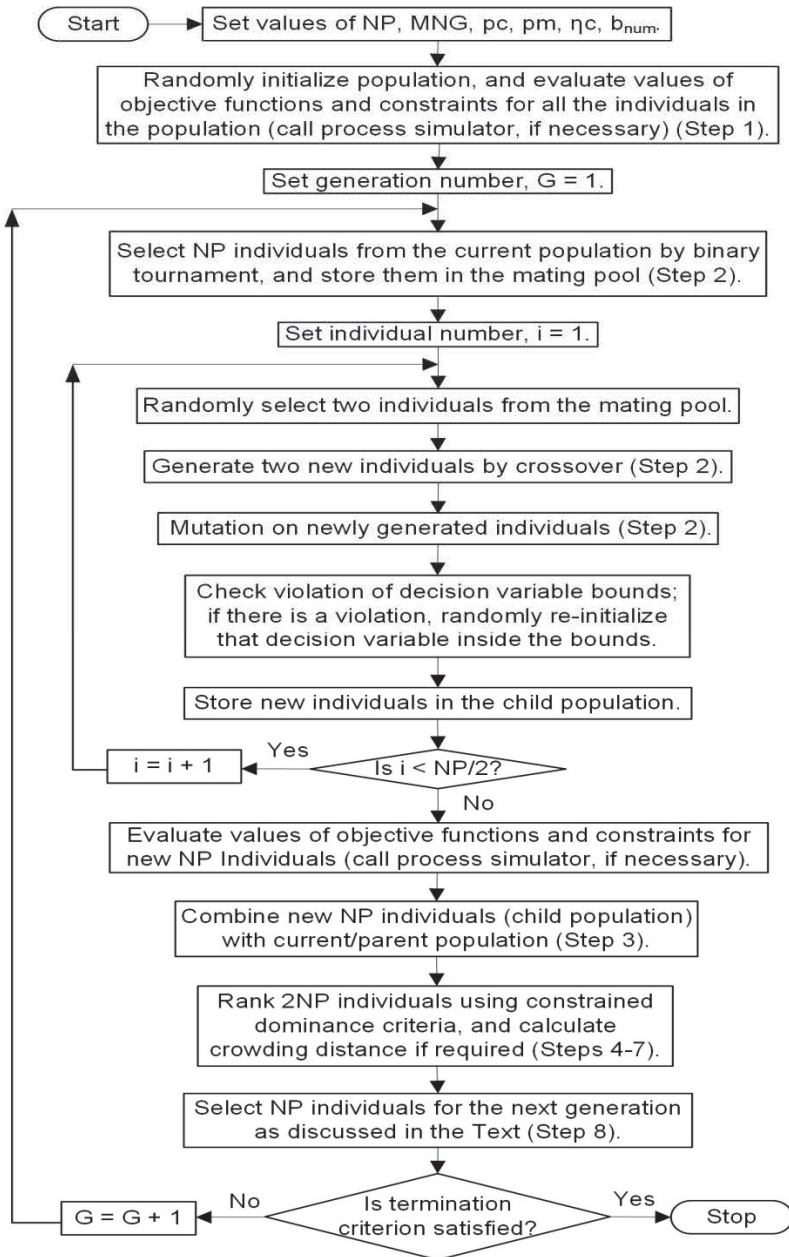
Fig. 16.1 A simplified flow-chart of the EMOO program; see Section 16.2 for details of steps in the flow-chart

The EMOO program and its Usage Guidelines can be obtained from the first author (shivomsharma.iitr@gmail.com) of this chapter. The NDS and PM programs, described later, can also be obtained from him. All three programs include important information for their usage.

16.3. Performance Metrics (PM)

In MOO, performance metrics such as generational distance and convergence metric are used to check convergence (i.e., closeness) of the non-dominated solutions obtained to the known/true Pareto-optimal front while some others such as spread and maximum spread are used to check the distribution of the non-dominated solutions obtained along the front. Further, performance metrics such as inverse generational distance and hyper-volume are used to evaluate both convergence and spread/distribution of the non-dominated solutions obtained. Some performance metrics use only one optimal set, called unary quality indicators, while other metrics, called binary quality indicators, quantitatively compare two approximation sets (Deb, 2001; Sharma and Rangaiah, 2013a).

Four widely-used performance metrics, implemented in the PM program in MS Excel, are described below. All these performance metrics are defined in the objective function space. For clarity, the phrase "non-dominated solutions" is used for the optimal solutions obtained by the MOO program, whereas the phrase "known/true Pareto-optimal front" refers to the analytical/approximate Pareto-optimal solutions/front.

(i) Generational Distance (GD) is used to evaluate the closeness of non-dominated solutions to the known/true Pareto-optimal front (van Veldhuizen and Lamont, 1998).

$$GD = \frac{1}{NP} \sqrt{\sum_{i=1}^{NP} d_i^2} \qquad (16.1)$$

Here, NP is the number of non-dominated solutions obtained by the MOO program, and d_i is the Euclidean distance of each of these solutions to its nearest point/solution on the known/true Pareto-optimal front.

(ii) Convergence Metric (CM) is also used to evaluate the closeness of non-dominated solutions to the known/true Pareto-optimal front (Zhou *et al.*, 2006).

$$CM = \frac{1}{NP} \sum_{i=1}^{NP} d_i \tag{16.2}$$

Thus, CM is simply the average of all d_i values as defined in Equation 16.1. In GD calculation, d_i values of all non-dominated solutions are squared, and so large d_i values play greater role in the summation under the square root.

(iii) Spread (SP) was introduced by Deb (2001) for bi-objective problems, to measure the distribution of non-dominated solutions obtained (say, set S). Its calculation requires the Euclidean distance between neighboring non-dominated solutions. SP also requires the Euclidean distance between the extreme non-dominated solutions (obtained by the MOO program) and the extreme solutions on the known/true Pareto-optimal front. Zhou *et al*. (2006) defined SP for more than two objectives, as follows.

$$SP = \frac{\sum_{m=1}^{M} \Delta(e_m,S) + \sum_{i=1}^{NP} |\Delta_i - \bar{\Delta}|}{\sum_{m=1}^{M} \Delta(e_m,S) + NP.\bar{\Delta}} \tag{16.3}$$

$$\Delta_i = \min \| S_i - S_j \|_2 \qquad j = 1, 2, \ldots, NP \text{ (except } i = j) \tag{16.4}$$

Here, M is the number of objective functions, and $\{e_1, e_2 \ldots, e_M\}$ are M extreme solutions on the known/true Pareto-optimal front. $\Delta(e_m, S)$ is the Euclidean distance between the extreme solution on the known/true Pareto-optimal front and the extreme non-dominated solution found, based on m^{th} objective. Δ_i is the Euclidean distance of ith non-dominated solution (S_i) to its nearest non-dominated solution (S_j), both found by the MOO program; and $\bar{\Delta}$ is the average of Δ_i of all non-dominated solutions.

(iv) In the objective function space, Inverse Generational Distance (IGD) is calculated between the known/true Pareto-optimal front and the non-dominated solutions obtained, as follows (Liu *et al*., 2009).

$$IGD = \frac{1}{NT} \sum_{i=1}^{NT} d_i' \tag{16.5}$$

Here, NT is the number of solutions in the known/true Pareto-optimal front. d_i' is the Euclidean distance of ith solution in the known/true Pareto-optimal front to its nearest non-dominated solution obtained by the MOO program. This is in contrast to d_i (which is the Euclidean distance of each non-dominated solution to its nearest solution on the known/true Pareto-optimal front) used in GD calculation.

16.3.1. *Modified Performance Metrics for Termination Criteria*

In case of application problems, the known/true Pareto-optimal front is not available in advance. Hence, original performance metrics cannot be

used to monitor the progress of the MOO search. Sharma and Rangaiah (2013a) modified the GD and SP to use only the non-dominated solutions obtained during the MOO search. As different objectives have different magnitudes in engineering applications, they should be normalized suitably before computing a performance metric, to avoid any bias. In this chapter, objectives are normalized using the extreme values of each objective of non-dominated solutions found in the current and previous generations of the stochastic search algorithm, and so each objective will be between 0 and 1. Then, modified GD (GD_m) and modified SP (SP_m) are calculated for the normalized values of objective functions.

GD_m is calculated between the non-dominated solutions obtained in the current and previous generations, using equation 16.1 and considering that non-dominated solutions obtained in the current generation are the known/true Pareto-optimal front. SP_m is calculated for the non-dominated solutions obtained in the current generation only using the following equations.

$$SP_m = \frac{\sum_{i=1}^{NP} |\Delta_i - \bar{\Delta}|}{NP\bar{\Delta}} \tag{16.6}$$

$$\Delta_i = \min \| S_i - S_j \|_2 \quad j = 1, 2, \ldots, NP \text{ (except } i = j) \tag{16.7}$$

Here, NP is the number of non-dominated solutions obtained in the current generation, and it can be lower than the population size used in the MOO program. The remaining symbols are same as those in equations 16.3 and 16.4.

16.4.   Termination Criteria

An effective and reliable termination criterion should terminate the stochastic search after detecting no improvement in the non-dominated solutions, to avoid unnecessary generations subsequently. Such a termination criterion, in addition to MNG, can save significant computational time for MOO of application problems. Since the known/true Pareto-optimal front is not available in advance for real-world applications, modified performance metrics can be used in the development of MOO search termination criteria. As mentioned in the previous section, Sharma and Rangaiah (2013a) modified GD and SP such that they require only non-dominated solutions obtained in different generations. Based on these, EMOO program has three termination criteria: Chi-Squared test based Termination Criterion (CSTC), Steady-

State Detection based Termination Criterion (SSDTC), and MNG. In the EMOO program, values of modified performance metrics are calculated from 21st generation onwards, as non-dominated solutions are unlikely to converge in the first 20 generations, and there are always fluctuations in performance metrics values in the early stage of search. Further, there should be at least four non-dominated solutions for calculating the modified performance metrics.

16.4.1. *Chi-Squared Test based Termination Criterion (CSTC)*

Sharma and Rangaiah (2013a) developed a MOO search termination criterion using chi-squared test on GD_m and SP_m values obtained in recent generations. The chi-squared test is performed on modified Performance Metric (PM) values in the latest λ generations, as follows. First, mean of performance metric (PM_m) is calculated by:

$$PM_m = \frac{\sum_{i=1}^{\lambda} PM_i}{\lambda} \tag{16.8}$$

Next, using the user-defined tolerance for standard deviation of PM (δ_{PM}), ratio of variance of PM values in the latest λ generations to the square of δ_{PM} is given by:

$$\chi^2 = \text{dof} \times \frac{\text{Variance of PM in } \lambda \text{ Generations}}{\delta_{PM}^2} \tag{16.9a}$$

$$= \text{dof} \times \frac{[\sum_{i=1}^{\lambda}(PM_i - PM_m)^2]/(\lambda-1)}{\delta_{PM}^2} \tag{16.9b}$$

Here, dof is the degree of freedom, which is equal to λ-1. Finally, the probability of chi-squared test supporting the hypothesis that variance of PM is lower than δ_{PM}^2, is found from the chi-squared distribution function in MS Excel:

$$p(PM) = \text{chi-squared}(\chi^2, \text{dof}) \tag{16.10}$$

Thus, chi-squared test checks whether the variance of PM in the latest λ generations is lower than the user-defined variance (δ_{PM}^2). The positive outcome of the test means PM is not changing significantly. This chapter uses the following values of parameters for chi-squared test: δ_{GD_m}= 0.0003, δ_{SP_m}= 0.1 and $\lambda = 10$. If the chi-squared test shows probability of more than 0.99 for both GD_m and SP_m individually, then MOO search is terminated. These values were found to be good for reliably

terminating the search, in the studies of Sharma and Rangaiah (2013a and 2014).

16.4.2. *Steady-State Detection based Termination Criterion (SSDTC)*

Rhinehart (2014) developed a steady-state detection technique to determine the convergence of a stochastic SOO method, and implemented it as a search termination criterion. The developed Steady-State Detection based Termination Criterion (SSDTC) for SOO performed with good precision and computational efficiency. Very recently, Wong *et al*. (2016) developed SSDTC for MOO, where steady-state detection technique is applied to values of GD_m and SP_m obtained in different generations.

In general, steady-state detection is based on variance ratio, where two variances are estimated using different methods on the same data set (Cao and Rhinehart, 1995). SSDTC procedure is initialized by finding the mean and variance of 10 values of the modified performance metrics (PM: GD_m and SP_m obtained from 21st to 30th generations). The mean value is used as the initial value of both PM_{prev} and $PM_{f,prev}$, whereas variance value is used as the initial value of $v^2_{f,prev}$, and twice that as the initial value of $\delta^2_{f,prev}$. These symbols are explained in the equations below, describing calculation steps from 31st generation onwards.

The following equation is used for an unbiased estimate of variance by the first method (i.e., for filtered values of the metric).

$$v^2_{f,curr} = \lambda_2\big(PM_{curr} - PM_{f,prev}\big)^2 + (1 - \lambda_2)v^2_{f,prev} \qquad (16.11)$$

Here, subscripts f, curr and prev refer to the filtered, current and previous values respectively; λ_2 is a user-defined filter coefficient. Then, the filtered performance metric is calculated using the following equation where λ_1 is a user-defined filter coefficient.

$$PM_{f,curr} = \lambda_1 PM_{curr} + (1 - \lambda_1)PM_{f,prev} \qquad (16.12)$$

Next, an unbiased estimate of variance by the second method (i.e., for the original or unfiltered values of the metric) is calculated using PM values without filtering:

$$\delta^2_{f,curr} = \lambda_3\big(PM_{curr} - PM_{prev}\big)^2 + (1 - \lambda_3)\delta^2_{f,prev} \qquad (16.13)$$

Here, λ_3 is a user-defined filter coefficient. Finally, ratio of the two estimates of variance (R_i) is calculated as (Cao and Rhinehart, 1995):

$$R_i = \frac{(2-\lambda_1)v_{f,curr}^2}{\delta_{f,curr}^2} \qquad (16.14)$$

In SSDTC for MOO, steady state (i.e., no significant changes in optimal solutions) is detected when R_i is below a user-specified critical value (R_{crit}). Wong *et al.* (2015) tested R_i for both GD_m and SP_m, and finally used R_i for GD_m only for MOO search termination. Accordingly, this chapter uses only GD_m along with the following parameter values for SSDTC: $\lambda_1 = \lambda_2 = \lambda_3 = 0.1$ and $R_{crit} = 0.9$, which were successfully used by Wong *et al.* (2016).

16.5. Simulation of Amine Absorption Process (AAP) for Natural Gas Sweetening

In natural gas, methane is the main component, and other hydrocarbons such as ethane, propane and butane are also present in smaller quantities. Further, water, CO_2 and H_2S are present as impurities in natural gas, and these have to be removed before its transportation. In the industry, AAP is commonly used to remove acid gases from natural gas (Niu and Rangaiah, 2014), and for CO_2 capture in power plants (Tock and Maréchal, 2014 and 2015). AAP for natural gas sweetening, shown in Fig. 16.2, is used to illustrate the application of the EMOO with termination criteria as well as NDS and PM programs, described later. This process is simulated in Aspen HYSYS v-8.7, using amine property package for vapor-liquor equilibrium predictions. Feed conditions and all stream data for one optimal solution are shown in Fig. 16.2.

In AAP (Fig. 16.2), natural gas enters the absorber at 55.16 bar and 30^0C. In the absorber, acid gases (CO_2 and H_2S) are absorbed in the di-ethanolamine (DEA) solution, whereas methane and other hydrocarbons remain in the gaseous stream. The gaseous mixture from the top of the absorber passes through a separator, in order to remove any trace of water. The liquid stream from the bottom of the absorber flows through a valve, to reduce pressure, and then to a flash tank to remove any vapor formed (off-gas). After that, the liquid stream exchanges heat with the bottom stream (regenerated DEA) of the regenerator for energy recovery, and then it enters the regenerator. In the regenerator, acid gases are removed as the vapor stream from the top, and the regenerated DEA as the bottom stream. The regenerated DEA, after cooling in the heat exchanger, is mixed with make-up water and further cooled before recycling to the absorber.
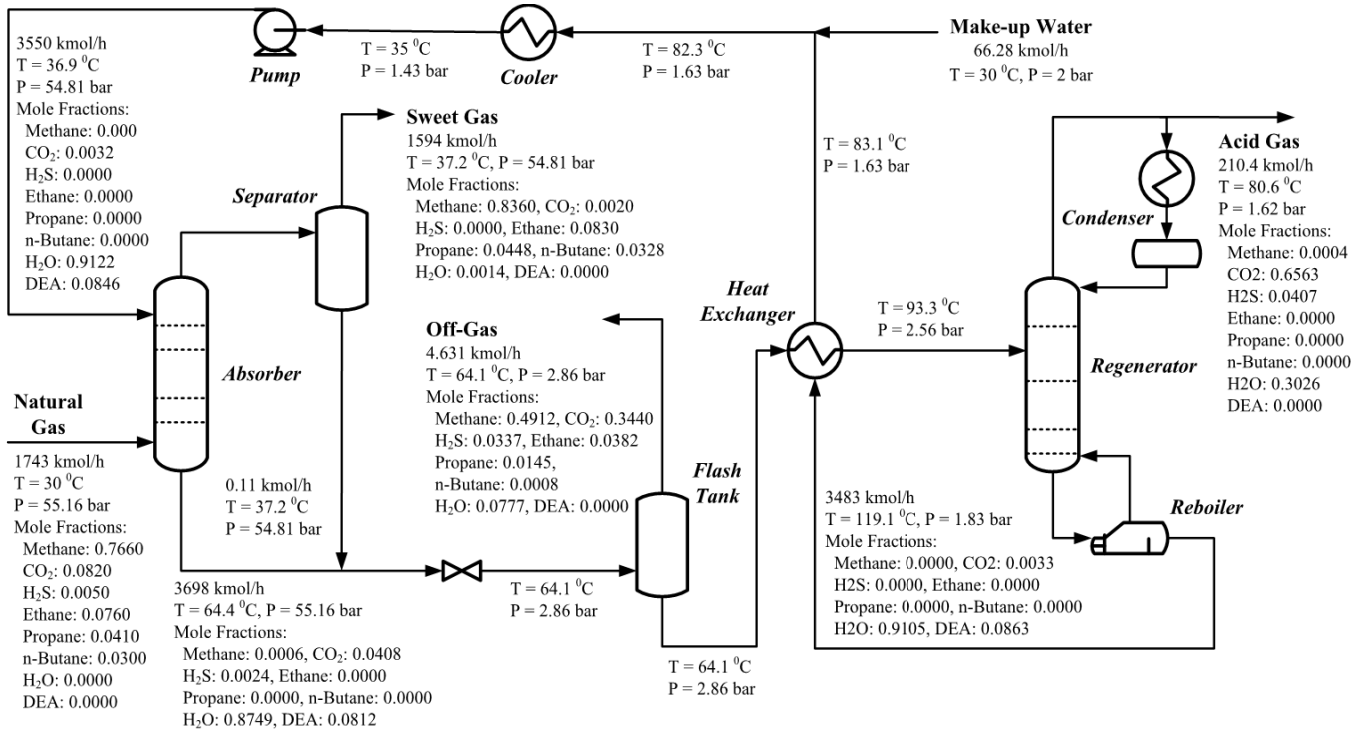
S. Sharma, G.P. Rangaiah and F. Maréchal

3550 kmol/h
T = 36.9 °C
P = 54.81 bar
Mole Fractions:
 Methane: 0.000
 CO₂: 0.0032
 H₂S: 0.0000
 Ethane: 0.0000
 Propane: 0.0000
 n-Butane: 0.0000
 H₂O: 0.9122
 DEA: 0.0846

Pump

T = 35 °C
P = 1.43 bar

Cooler

T = 82.3 °C
P = 1.63 bar

Make-up Water
66.28 kmol/h
T = 30 °C, P = 2 bar

Separator

Sweet Gas
1594 kmol/h
T = 37.2 °C, P = 54.81 bar
Mole Fractions:
 Methane: 0.8360, CO₂: 0.0020
 H₂S: 0.0000, Ethane: 0.0830
 Propane: 0.0448, n-Butane: 0.0328
 H₂O: 0.0014, DEA: 0.0000

T = 83.1 °C
P = 1.63 bar

Acid Gas
210.4 kmol/h
T = 80.6 °C
P = 1.62 bar
Mole Fractions:
 Methane: 0.0004
 CO2: 0.6563
 H2S: 0.0407
 Ethane: 0.0000
 Propane: 0.0000
 n-Butane: 0.0000
 H2O: 0.3026
 DEA: 0.0000

Condenser

Absorber

Off-Gas
4.631 kmol/h
T = 64.1 °C, P = 2.86 bar
Mole Fractions:
 Methane: 0.4912, CO₂: 0.3440
 H₂S: 0.0337, Ethane: 0.0382
 Propane: 0.0145,
 n-Butane: 0.0008
 H₂O: 0.0777, DEA: 0.0000

Heat Exchanger

T = 93.3 °C
P = 2.56 bar

Regenerator

Reboiler

Natural Gas
1743 kmol/h
T = 30 °C
P = 55.16 bar
Mole Fractions:
 Methane: 0.7660
 CO₂: 0.0820
 H₂S: 0.0050
 Ethane: 0.0760
 Propane: 0.0410
 n-Butane: 0.0300
 H₂O: 0.0000
 DEA: 0.0000

0.11 kmol/h
T = 37.2 °C
P = 54.81 bar

Flash Tank

3483 kmol/h
T = 119.1 °C, P = 1.83 bar
Mole Fractions:
 Methane: 0.0000, CO2: 0.0033
 H2S: 0.0000, Ethane: 0.0000
 Propane: 0.0000, n-Butane: 0.0000
 H2O: 0.9105, DEA: 0.0863

3698 kmol/h
T = 64.4 °C, P = 55.16 bar
Mole Fractions:
 Methane: 0.0006, CO₂: 0.0408
 H₂S: 0.0024, Ethane: 0.0000
 Propane: 0.0000, n-Butane: 0.0000
 H₂O: 0.8749, DEA: 0.0812

T = 64.1 °C
P = 2.86 bar

T = 64.1 °C
P = 2.86 bar

Fig. 16.2 A schematic of amine absorption process for acid gas removal from natural gas; stream data correspond to one selected optimal solution in Figure 16.4(a)

16.6.   MOO of Amine Absorption Process

Table 16.1 presents the MOO problem formulated for AAP for natural gas sweetening. Here, total capital cost is considered as one of the objectives. Operating cost, which includes cooling water, make-up water, steam and electricity costs, is considered as the second objective in the optimization problem. Five important design and operational parameters are the decision variables; of these four are integer variables. Table 16.1 also presents the ranges of all decision variables; these ranges are based on preliminary sensitivity analysis of the process (e.g., to ensure convergence of simulation). In order to fulfill the quality requirements of natural gas, several constraints are imposed on the sweet gas. A constraint for maximum concentration of CH_4 in acid gas is also included, to avoid loss of hydrocarbons in the acid gas stream. Finally, logarithmic mean temperature difference of 20 ^0C is maintained (i.e., LMTD > 20 ^0C), for heat exchanger, cooler, reboiler and condenser.

Table 16.1 MOO problem formulation for amine absorption process for acid gases removal from natural gas

Objective Functions		
Objective function 1 ($)	Min. Total Capital Cost (TCC)	
Objective function 2 ($/y)	Min. Annual Operating Cost (AOC)	
Decision Variables	Lower Bound	Upper Bound
No of theoretical stages in the absorber	18	22
Pressure of flash tank (bar)	2	4
No of theoretical stages in the regenerator	16	20
Feed stage of regenerator	3	8
Reflux ratio of regenerator	0.5	0.6
Constraints		
Sweet gas flow rate (kmol/h)	>	1590.0
CO_2 in sweet gas (mole fraction)	<	0.005
H_2S in sweet gas (mg/m^3)	<	5.5
H_2O in sweet gas (mg/m^3)	<	80.0
Acid gas flow rate (kmol/h)	>	210.0
CH_4 in acid gas (mole fraction)	<	0.01
LMTD (of heat exchanger, cooler, reboiler or condenser; ^0C) >		20.0

Capital cost of different equipment in AAP is estimated using correlations and data in Turton *et al*. (2009). The Chemical Engineering

Plant Cost Index (CEPCI) value of 600 is used for capital cost estimation. Overall heat transfer coefficient for heat exchanger, cooler, condenser or reboiler is assumed to be 300 W/(m^2.K). Efficiency of stages in the absorber and regenerator is assumed to be 0.75. Costs of cooling water (= 0.0000148 \$/kg), make-up/process water (= 0.000067 \$/kg), low pressure steam (= 0.02929 \$/kg; P = 5 barg and T = 160 ^{0}C) and electricity (0.06 \$/kWh) are taken from Turton *et al.* (2009). Finally, operating time of AAP process is assumed to be 8000 hours/year.

As stated earlier, the EMOO program has been developed in MS Excel; it is interfaced with AAP simulated in Aspen HYSYS via VBA. Fig. 16.3 shows the structure of this interfacing. As shown in this figure, the EMOO program provides a new set of decision variables, which is passed to Aspen HYSYS via VBA. After the convergence of Aspen HYSYS simulation, data required for the calculation of objectives and constraints are transferred from Aspen HYSYS to MS Excel. Values of objective functions and constraints calculated in MS Excel are used by the NSGA-II algorithm in Fig. 16.3.
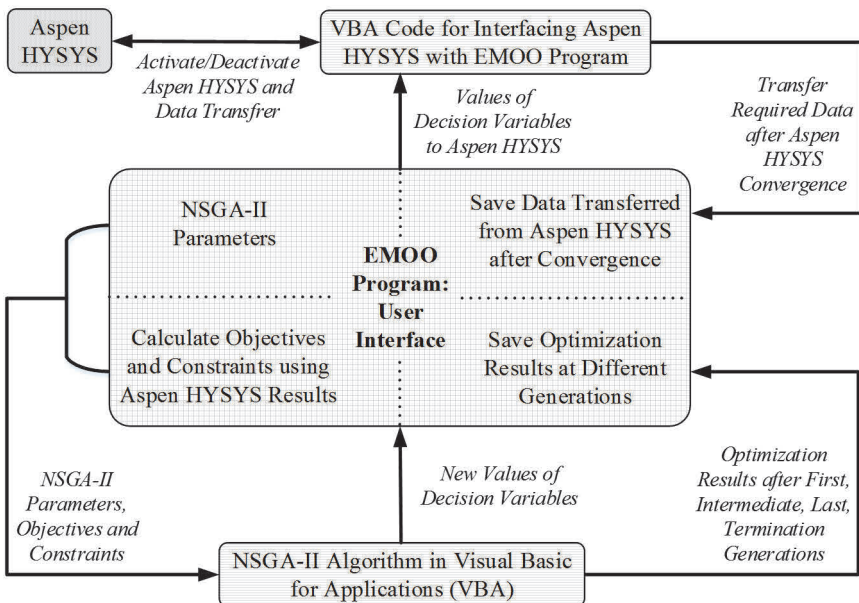
Fig. 16.3 Interfacing of the EMOO program with Aspen HYSYS via VBA

In order to reduce the computation time, Aspen HYSYS simulation has to be put on hold and then values of decision variables are passed to the simulation file. After that, Aspen HYSYS simulation is activated. If the process simulation fails to converge for a particular set of decision variables, then worst values should be assigned to objectives and constraints, and that particular solution will be eliminated from the population during the next generation of the EMOO program. Further, the unconverged simulation file should be closed without saving, and the previously saved file should be opened before calling the simulation file for a new set of decision variables. More details on the interfacing of MS Excel with Aspen HYSYS can be found in Sharma and Rangaiah (2016).

Fig. 16.4(a) presents the non-dominated solutions obtained for AAP using the binary-coded NSGA-II available in the EMOO program. These results are obtained with NP = 100, crossover probability (p_c) for uniform crossover = 0.9 and mutation probability (p_m) for bit-wise mutation = 0.1. It can be seen that both the termination criteria in the EMOO program stop the MOO search well before the MNG (= 100), and the non-dominated solutions obtained after termination generations (36 for CSTC and 41 for SSDTC) and MNG are similar. Hence, inclusion of termination criteria based on search progress can significantly save the computation time.

Optimal number of stages in the absorber and regenerator is respectively 18 and 16 whereas the optimum feed stage of the regenerator is 8, for all non-dominated solutions (Fig. 16.4). Further, reflux ratio is close to its lower bound (= 0.5), for all non-dominated solutions. The reason for these values is that each of these decision variables affects both the objectives in the same direction. The trend of the non-dominated solutions is mainly due to flash tank pressure. In order to ensure sufficiently large driving force at the both ends of the heat exchanger, temperature of feed stream to the regenerator is fixed at 93.3 ^{0}C. Hence, the feed stream to the regenerator has higher vapor fraction at a lower value of flash tank pressure. This decreases regenerator reboiler duty for a lower value of flash tank pressure. As the regenerator reboiler duty accounts for ~95% of operating cost, annual operating cost decreases with the flash tank pressure. Further, cost of the heat exchanger is higher for a lower value of flash tank pressure, and vice versa. Hence, total capital cost increases and annual operating cost decreases with decrease in the flash tank pressure (Fig. 16.4).

Fig. 16.5(a) shows the non-dominated solutions obtained for AAP using the real-coded NSGA-II in the EMOO program. These results are obtained with NP = 100, η_c = 5 and b_{num} = 4 (Wong *et al*., 2016). The MOO search was terminated by CSTC after 30 generations, and the non-dominated solutions obtained after 30 generations are close to those obtained after MNG (= 100). The SSDTC was able to terminate the search after 72 generations, and the non-dominated solutions obtained after 72 and 100 generations are similar. The trend of the non-dominated solutions is mainly due to flash tank outlet pressure. For all the non-dominated solutions, optimal values of number of stages in absorber and regenerator are respectively 18 and 16, whereas 8 is the optimum feed stage for regenerator. Reflux ratio is close to its lower bound (= 0.5), for all the non-dominated solutions (Fig. 16.5b-f). The trends/values in Fig. 16.5 are similar as those in Fig. 16.4. In general, termination criteria in the EMOO program have good performance for MOO of AAP for acid gases removal, which shows their applicability to industrial optimization problems.

There is still some scope for improving the optimal solutions by changing bounds of decision variables suitably while ensuring convergence of the process simulation for the expanded ranges of decision variables. In the optimization problem definition, bounds of decision variables play an important role by restricting the search space, which has a techno-physical meaning. Hence, decision variable bounds are used to limit the search space, where correlations and process models are valid. In particular, this is the case for correlations and heuristic rules used in the sizing of process units and choice of materials (corrosiveness, temperature and pressure). The choice of specification values in simulation and the ranges for decision variables are critical tasks for engineers when stating the optimization problem. Good ranges for decision variables lead to identification of realistic optimal solution(s). The identification of decision variables whose optimal values are at lower/upper bound gives good engineering insight, and also defines challenges for engineers by indicating the direction of future technology development. Note that, in mathematical programming, Lagrange multipliers give the sensitivity of active decision variables (i.e., those at the bound at the optimum) on the objective.
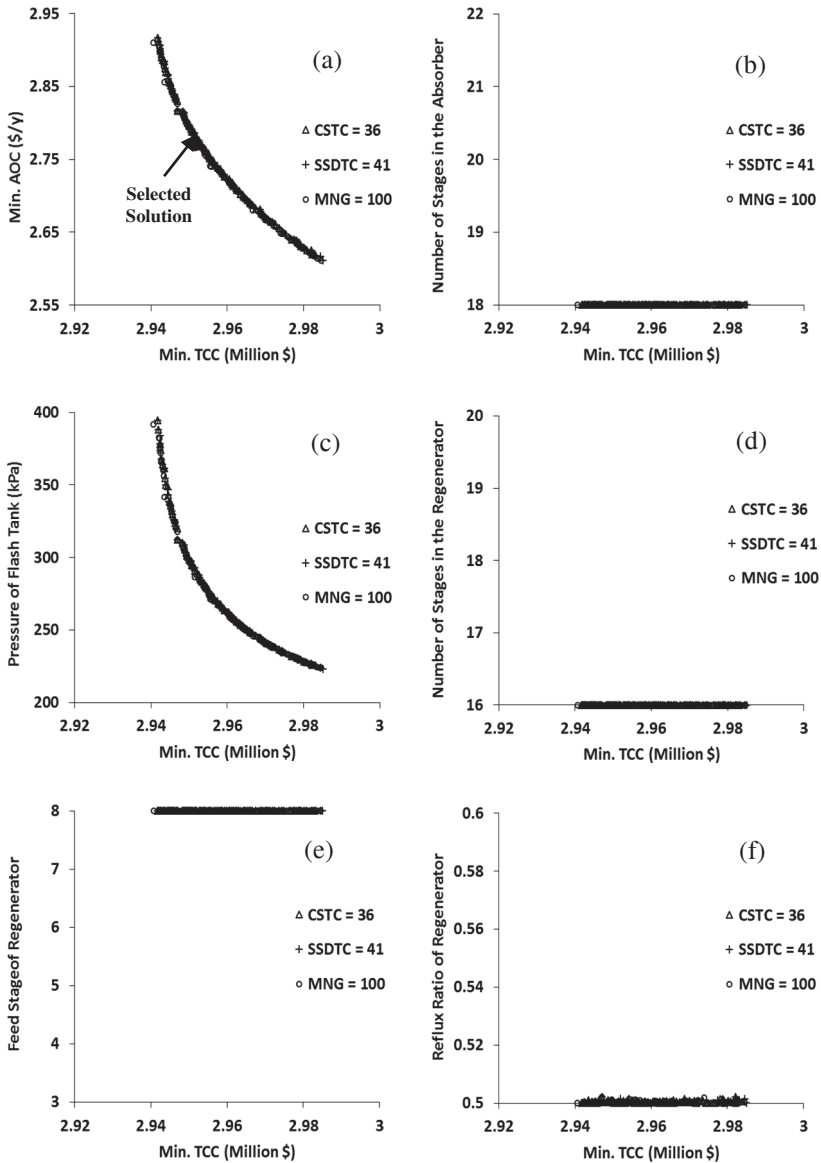
Fig. 16.4 MOO results for amine absorption process for natural gas sweetening using the binary-coded NSGA-II in the EMOO program; for this figure in color, see the supplementary material on the book website.
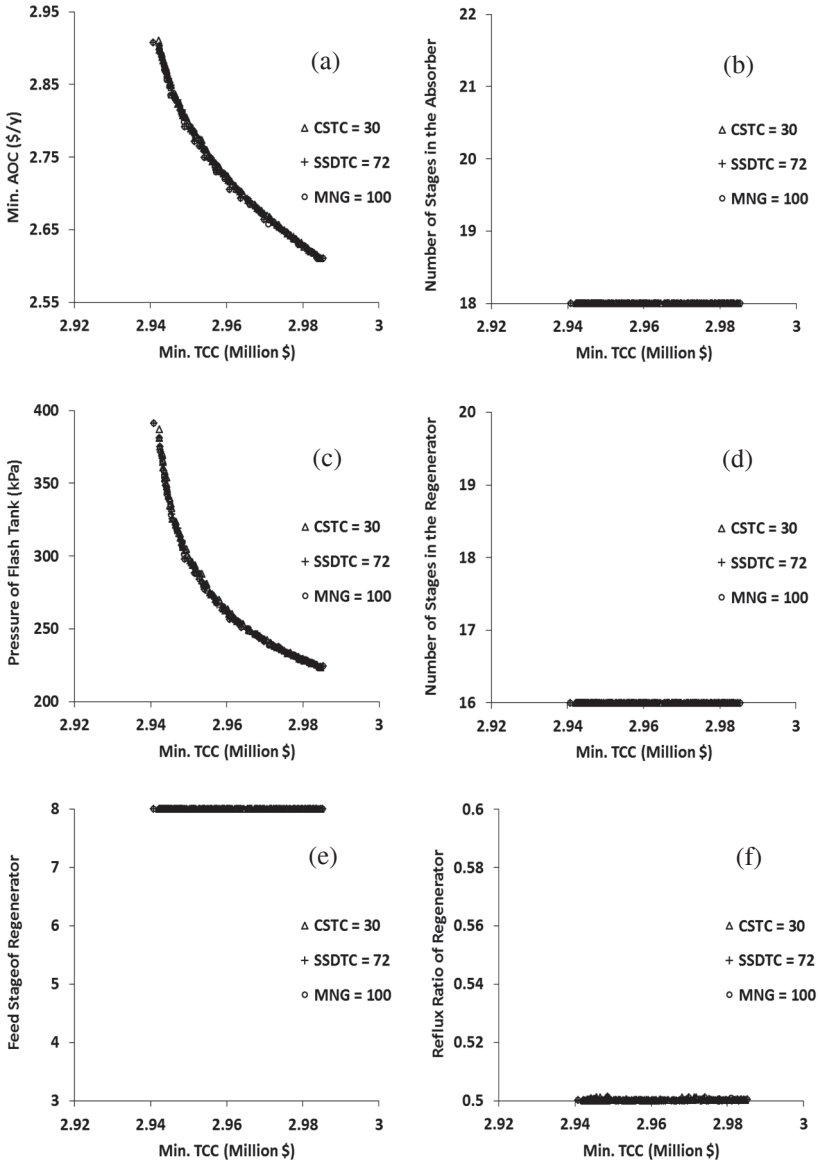
Fig. 16.5 MOO results for amine absorption process for natural gas sweetening using the real-coded NSGA-II in the EMOO program; this figure in color is available in the supplementary material on the book website.

Figs. 16.6(a), 6(b) and 6(c) compare the non-dominated solutions obtained using the binary- and real-coded NSGA-II in the EMOO program, after search termination by CSTC, SSDTC and MNG, respectively. Thus, for AAP, optimal values of objectives and decision variables obtained using the binary-coded NSGA-II are comparable to those using the real-coded NSGA-II in the EMOO program.
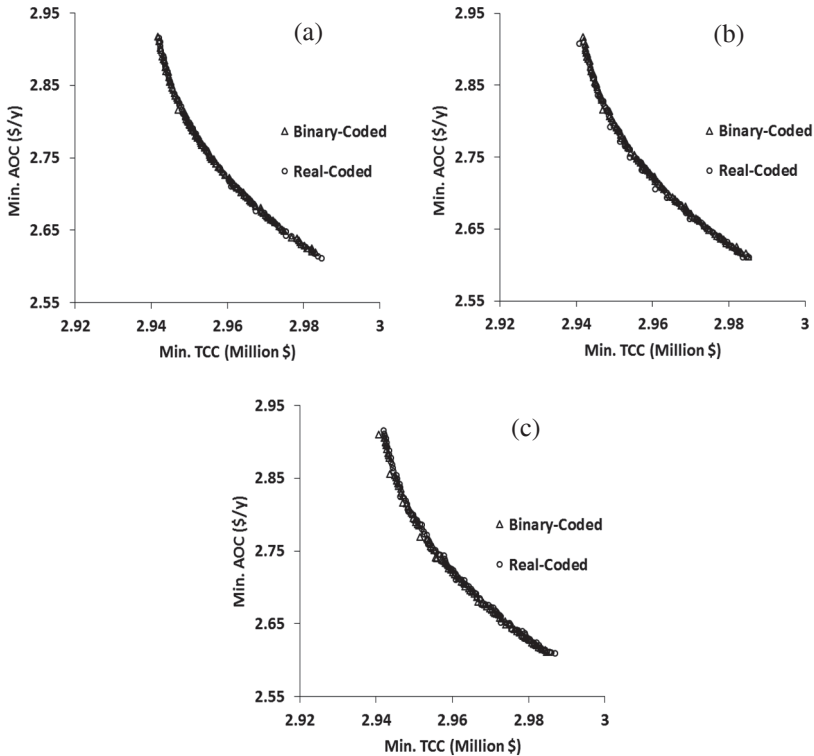
Fig. 16.6 Non-dominated solutions obtained using the binary- and real-coded NSGA-II in the EMOO program, after search termination by (a) CSTC, (b) SSDTC, and (b) MNG; for this figure in color, see the supplementary material on the book website.

16.7.   Non-dominated Sorting (NDS) Program in MS Excel

In order to evaluate the qualities of non-dominated solutions obtained by a stochastic MOO program, they have to be compared with the best possible solutions of that optimization problem. Mathematical MOO

problems can sometimes be solved analytically, and so their analytical solutions can be used for assessing the quality of obtained solutions using a stochastic MOO program. These situations arise for assessing the improvements in new MOO algorithms. Optimization problems for engineering applications cannot be solved analytically, and so their best solutions are unknown. (Note that, whenever possible, solving a problem analytically is better than solving it numerically as the latter brings issues such as numerical errors and convergence.) Hence, to find their best solutions, it is suggested to solve the MOO problem of the engineering application many times (say, 5 or many more times depending on the computational effort required) for a very large MNG (e.g., 1000 or more) using a stochastic MOO program. Then, combine the non-dominated solutions obtained in different runs and sort them to find the known/true Pareto-optimal front, which can then be used to calculate the desired performance metrics.

To find the known/true Pareto-optimal front based on the results from many runs of a MOO program (such as EMOO), NDS program in MS Excel is developed. In this, all non-dominated solutions obtained in different runs are combined (i.e., copied into the 'Input' worksheet in the NDS program), and then non-dominated sorting is performed as described in Steps 4 to 8 of NSGA-II algorithm presented in Section 16.2. These calculation steps are coded using VBA within MS Excel. The first Pareto front found from this non-dominated sorting is selected as the known/true Pareto-optimal front for that particular application problem. If this has more non-dominated solutions than required by the user, then crowding distance calculations are performed to select the least crowded non-dominated solutions from the first Pareto front (or the known/true Pareto-optimal front). In the NDS program, user can provide the optimal solutions from different runs on the 'Input' worksheet of NDS program, and then can get the results on the 'Output' worksheet.

For the AAP optimized in the previous section, there are 100 non-dominated solutions in each run, and in total 500 solutions from 5 runs (shown in Fig. 16.7a). Fig. 16.7(b) presents the known/true Pareto-optimal front for AAP, which is obtained by consolidating solutions obtained from 5 different runs of the EMOO program. Sorting these solutions gave 124 optimal solutions in the first/best Pareto-optimal front (shown in Fig. 16.7b). In case user specifies only 100 non-dominated solutions, then crowding distance calculations are performed, and the known/true Pareto-optimal front with 100 solutions is shown in Fig.

16.7(c). Interested reader can obtain the NDS program with these results from the first author (shivomsharma.iitr@gmail.com); this program contains general instructions that should be followed carefully for using it successfully.
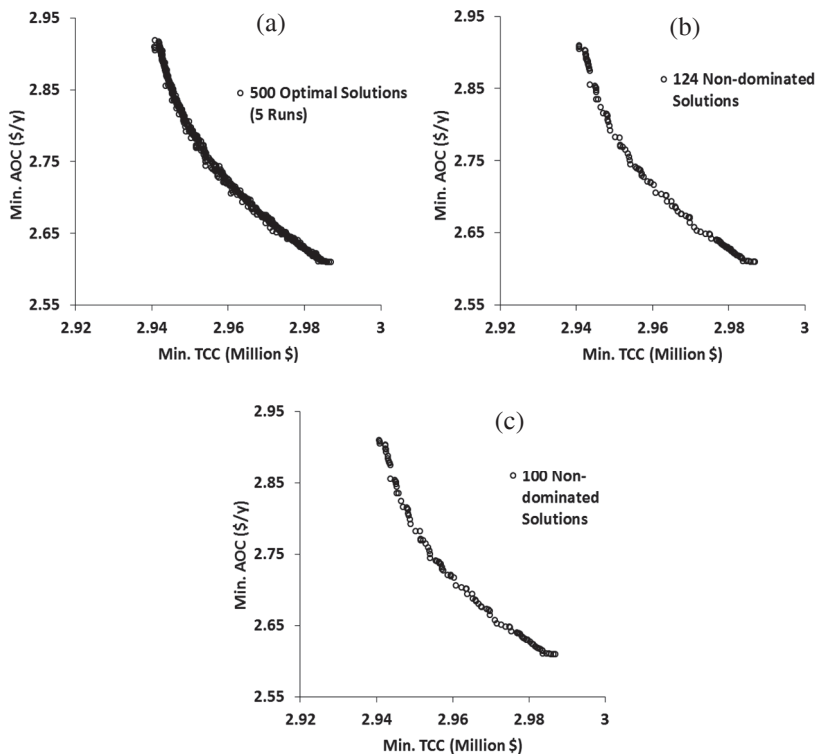

Fig.16.7 (a) Optimal solutions obtained in 5 different runs of the EMOO program (2 runs of binary-coded NSGA-II and 3 runs of real-coded NSGA-II) after MNG, (b) all 124 non-dominated solutions in the first/best Pareto front, and (c) 100 least crowded non-dominated solutions in the first/best Pareto front; for this figure in color, see the supplementary material on the book website.

16.8.   Performance Metrics (PM) Program in MS Excel

Non-dominated solutions obtained using an MOO program can be shown in plots such as Figs. 16.4(a) and 16.5(a). Although useful for presentation and comprehending the optimal solutions, they are not suitable for quantitative assessment of non-dominated solutions obtained

at different generations, in runs and/or programs. Hence, multi-objective performance metrics are employed to evaluate the quality of non-dominated solutions obtained; for this, the known/true Pareto-optimal front, obtained analytically from the literature or from many runs followed by using the NDS program (described in the previous section), is used as the reference.

PM program in MS Excel has been developed for calculating GD, CM, IGD and SP between the non-dominated solutions obtained and the known/true Pareto-optimal front. These performance metrics are described in Section 16.3. PM program provides two sets of performance metric values: (1) based on the actual values of objective functions, and (2) based on the normalized values of objective functions. For the later set, the non-dominated solutions obtained and known/true Pareto-optimal solutions are normalized between 0 and 1, using the extreme values of objectives in the known/true Pareto-optimal front.

Table 16.2 presents values of GD, CM, IGD and SP for non-dominated solutions obtained for AAP after MNG using binary- and real-coded NSGA-II. It includes values of these performance metrics based on actual values of objective functions, and also based on normalized values of objective functions. It is clear from Table 16.2 that both binary- and real-coded NSGA-II have comparable performance for optimizing AAP for natural gas sweetening. One can see the large effect of normalization on GD, CM and IGD, and not much on SP. This may not be important for comparing two different algorithms or runs on one application (as in Table 16.2) but it is important for assessing results from more than one application. Interested readers can obtain PM program with the results for AAP from the first author (shivomsharma.iitr@gmail.com); this program includes important information for its usage.

Table 16.2 Values of performance metrics for non-dominated solutions obtained after MNG for one run of binary- and real-coded NSGA-II (Figs. 16.4a and 16.5a); known/true Pareto-optimal front in Fig. 16.7(b) is used as the reference solution; OF: objective function

	Binary-coded NSGA-II		Real-coded NSGA-II	
	Using Actual Values of OF	Using Normalized Values OF	Using Actual Values of OF	Using Normalized Values OF
GD	172.2106	0.0014	208.7303	0.0011
CM	114.1773	0.0011	104.8083	0.0008
IGD	1240.9990	0.0104	1169.9053	0.0076
SP	0.4640	0.3443	0.5106	0.4141

16.9.   Conclusions

This chapter describes methodologies of three programs, developed in MS Excel, useful for MOO and for analysis of optimal results. The EMOO program can be used to generate the non-dominated solutions for multi-objective problems. It has two termination criteria based on the search progress (besides MNG), and the user can use one of them to save computation time. The NDS program can be used to obtain the known/ true Pareto-optimal front for application problems. For this, the application problem has to be solved many times using a program such as EMOO for sufficiently large number of generations, and then NDS program can be used to obtain the known/true Pareto-optimal front from the solutions obtained in different runs. The PM program, also developed in MS Excel, is used to calculate values of four important multi-objective performance metrics between the non-dominated solutions obtained by a MOO program and the known/true Pareto-optimal front. To illustrate the use of the three programs described, AAP for natural gas sweetening is simulated and optimized for total capital cost and annual operating cost simultaneously, using the EMOO program. Finally, NDS and PM programs are employed to analyze the optimization results obtained for AAP process.

Acknowledgement

Nomenclature

Abbreviations

AAP	Amine Absorption Process
CM	Convergence Metric
CEPCI	Chemical Engineering Plant Cost Index
CSTC	Chi-Squared Test based Termination Criterion
DEA	Di-ethanolamine
EMOO	Excel based Multi-Objective Optimization
GA	Genetic Algorithms

GD	Generational Distance
IGD	Inverse Generational Distance
LMTD	Log-Mean Temperature Difference
MNG	Maximum Number of Generations
MOO	Multi-Objective Optimization
NDS	Non-Dominated Sorting
NSGA	Non-Dominated Sorting Genetic Algorithm
OF	Objective Function
PM	Performance Metric
SOO	Single Objective Optimization
SP	Spread
SSDTC	Steady-Stage Detection based Termination Criterion
TCC	Total Capital Cost
VBA	Visual Basic for Applications

References

Cao S. and Rhinehart R. R. (1995), *An Efficient Method for On-line Identification of Steady State*, J. Process Control, 5(6), pp. 363-374.

Cheah K. S. and Rangaiah G. P. (2009), *Multi-objective Optimization in Food Engineering*, In Erdogdu F. (editor), Optimization in Food Engineering, Taylor and Francis/CRC Press, Boca Raton.

Coello Coello, C. A., Lamont, G. B. and van Veldhuizen, D. A. (2007), Evolutionary Algorithms for Solving Multi-objective Problems, Springer, Berlin/Heidelberg, 2nd ed.

Deb K. (2001), Multi-Objective Optimization using Evolutionary Algorithms, John Wiley & Sons, New York.

Deb K., Pratap A., Agarwal S. and Meyarivan T. (2002), *A Fast and Elitist Multi-objective Genetic Algorithm: NSGA-II*, IEEE Transactions on Evolutionary Computation, 6(2), pp. 182-197.

Liu M., Zou X., Chen Y. and Wu Z. (2009), *Performance Assessment of DMOEA-DD with CEC 2009 MOEA Competition Test Instances*, CEC Special Session on the Performance Assessment of Multi-objective Optimization Algorithms.

Niu, M. W. and Rangaiah G. P. (2014), *Retrofitting Amine Absorption Process for Natural Gas Sweetening via Hybridization with Membrane Separation*, International Journal of Greenhouse Gas Control, 29, pp. 221-230.

Rangaiah G. P., Sharma S. and Sreepathi B. K. (2015), *Multi-objective Optimization for the Design and Operation of Energy Efficient Chemical Processes and Power Generation*, Current Opinion in Chemical Engineering, 10, pp. 49-62.

Rhinehart, R. R. (2014), *Convergence Criterion in Optimization of Stochastic Processes*, Computers and Chemical Engineering, 68, pp.1-6.

Sharma S., Rangaiah G. P. and Cheah K. S. (2012), *Multi-objective Optimization using MS Excel with an Application to Design a Falling Film Evaporator System*, Food and Bioproducts Processing, 90(2), pp. 123-134.

Sharma S. and Rangaiah G. P. (2013a), *An Improved Multi-Objective Differential Evolution with a Termination Criterion for Optimizing Chemical Processes*, Computers & Chemical Engineering, 56, pp. 155-173.

Sharma S. and Rangaiah G. P. (2013b), *Multi-objective Optimization Applications in Chemical Engineering*, In Rangaiah G. P. and Bonilla-Petriciolet, A. (editors), Multi-Objective Optimization in Chemical Engineering: Developments and Applications, Wiley, Chichester.

Sharma S. and Rangaiah G. P. (2014), *Hybrid Approach for Multi-Objective Optimization and its Applications to Process Engineering Problems*, In Jayaraman V. and Siarry P. (editors), Recent Advances in Applications of Metaheuristics in Process Engineering, Springer, Heidelberg.

Sharma S. and Rangaiah G. P. (2016), *Mathematical Modeling, Simulation and Optimization for Process Design*, In Rangaiah G. P. (editor), Chemical Process Retrofitting and Revamping: Techniques and Applications, Wiley, Chichester.

Srinivas N. and Deb K. (1994), *Multi-objective Optimization using Non-Dominated Sorting in Genetic Algorithm*, Evolutionary Computation, 2(3), pp. 221-248.

Tock L. and Maréchal F. (2014), *Process Design Optimization Strategy to Develop Energy and Cost Correlations of CO_2 Capture Processes*, Computers & Chemical Engineering, 61, pp. 51-58.

Tock L. and Maréchal F. (2015), *Environomic Optimal Design of Power Plants with CO2 Capture*, International Journal of Greenhouse Gas Control, 39, pp. 245-255.

Trautmann H., Wagner T., Naujoks B., Preuss M. and Mehnen J. (2009), *Statistical Methods for Convergence Detection of Multi-Objective Evolutionary Algorithms*, Evolutionary Computation, 17(4), pp. 493-509.

Turton R., Bailie R. C., Whiting W. B. and Shaeiwitz J. A. (2009), Analysis, Synthesis and Design of Chemical Processes, 3rd ed., Prentice Hall, New York.

van Veldhuizen D. A. and Lamont G. B. (1998), *Evolutionary Computation and Convergence to a Pareto Front*. (citeseerx.ist.psu.edu/viewdoc/summary? doi=10.1.1.42.7224).

Wong J. Y. Q., Sharma S. and Rangaiah G. P. (2016), *Design of Shell-and-Tube Heat Exchangers for Multiple Objectives using Elitist Non-Dominated Sorting Genetic Algorithm with Termination Criteria*, Applied Thermal Engineering, 93, pp. 888-899.

Zhou A., Jin Y. and Zhang Q. (2006), *Combining Model-Based and Generics-Based Offspring Generation for Multi-Objective Optimization using a Convergence Criterion*, IEEE Congress on Evolutionary Computation, pp. 3234-3241.

Exercises

For the following exercises, Aspen HYSYS simulation file for AAP as well as EMOO, NDS and PM programs (in MS Excel) can be obtained from the first author of this chapter (shivomsharma.iitr@gmail.com).

1. In this chapter, natural gas flow rate, F = 1743 kmol/h. Optimize AAP considering two different feed flow rates (e.g., F/2 and F) for

total capital cost and annual operating cost. Assess the results obtained for the benefits of economy of scale.

2. Assume higher mole fraction (than that shown in Fig. 16.2) of CO_2 and H_2S in the natural gas, and then optimize the AAP for natural gas flow rate of 1743 kmol/h, for total capital cost and annual operating cost. Based on the optimal results, discuss the effect of increased concentration of CO_2 and H_2S on the capital and operating costs.

3. Explore tradeoff among total capital cost, annual operating cost and hydrocarbon loss (i.e., methane, ethane, propane and n-butane in acid gas and off-gas) by optimizing AAP for three objectives.

4. For each of the above exercises, use NDS and PM programs to (1) obtain the true/known Pareto-optimal front, and (2) calculate values of multi-objective performance metrics.