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Improved Constraint Handling Technique for Multi-Objective Optimization with Application to Two Fermentation Processes

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5.1 Introduction

Multi-objective optimization (MOO) has had numerous chemical engineering applications (Masuduzzaman and Rangaiah, 2009; see also Chapter 3 in this book). Application problems often have constraints besides bounds on decision variables; these constraints arise from design equations (such as mass and energy balances), equipment limitations (such as size) and operation requirements (such as temperature limit for safe operation). For example, Guria *et al.* (2005) have optimized the reverse osmosis process for multiple objectives. Here, solvent and solute mass balances around the reverse osmosis module have to be solved for calculating objective functions. For each set of decision variable values, Guria *et al.* (2005) have solved these model equations; this strategy is referred to as the sequential solution approach; further, they used the penalty function approach for handling inequality constraints. An alternative strategy is to treat the model equations as equality constraints in the optimization problem; this strategy is referred to as simultaneous solution approach.

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The mathematical form of a constrained MOO optimization problem is as follows:

$$\text{Minimize} \quad \{f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots f_k(\mathbf{x})\} \tag{5.1}$$

$$\text{Subject to} \quad \mathbf{x}^L \leq \mathbf{x} \leq \mathbf{x}^U \tag{5.2}$$

$$\mathbf{h}(\mathbf{x}) = \mathbf{0} \tag{5.3}$$

$$\mathbf{g}(\mathbf{x}) \leq \mathbf{0} \tag{5.4}$$

Here $f_1, f_2, \ldots, f_k$ are k number of objective functions; $\mathbf{x}$ is the vector of n decision variables; $\mathbf{x}^L$ and $\mathbf{x}^U$ are respectively vectors of lower and upper bounds on decision variables; and **h** and **g** are the set of n_e equality and n_i inequality constraints respectively.

Many algorithms have been proposed to solve MOO problems; examples of these algorithms are the elitist non-dominated sorting genetic algorithm (NSGA-II; Deb *et al.*, 2002), strength Pareto evolutionary algorithm (SPEA2; Zitzler *et al.*, 2001), multi-objective particle swarm optimization (MO-PSO; Coello Coello and Salazar Lechuga, 2002) and multi-objective differential evolution (MODE). Originally, MOO algorithms were developed and studied for solving unconstrained optimization problems (i.e., with bounds on decision variables but without any inequality or equality constraints). Later, to solve constrained MOO problems, several constraint-handling techniques were developed and incorporated in the MOO algorithms.

Coello Coello (2002) summarized constraint handling methods utilized in evolutionary algorithms under five main categories: (i) penalty function approach, (ii) separation of constraints and objectives, (iii) special representation, (iv) repair algorithms, and (v) hybrid methods. The penalty function approach penalizes objective functions (e.g., it increases their values by adding penalty terms, in case of minimization of objectives), based on the extent of constraint violation; it is simple in concept and has been popular. However, the difficulty in using this approach is the selection of a suitable penalty factor value for different problems. If the penalty factor value is not appropriate, then the optimization algorithm may converge to either a non-optimal feasible solution or an infeasible solution. Penalty function approach is divided into several subcategories (e.g., static, dynamic, adaptive, co-evolutionary, etc.) based on the method of penalty factor handling. If the objective function value cannot be computed in the infeasible search space for some reason, then the penalty function approach cannot be used for solving such constrained optimization problems. For example, mathematical functions such as logarithms and/or square roots, present in the objectives, cannot be evaluated for negative values of their arguments. If values of objective functions cannot be calculated or a process simulator does not converge for a particular set of decision variable values (i.e., potential solution), then the worst value for each objective can be given. This solution, then, is very unlikely to be selected for the subsequent generation.

Deb *et al.* (2002) proposed feasibility approach for handling inequality constraints, which considers the constraints and objectives separately. It selects a feasible solution over an infeasible solution during the selection step in the generations. Constraint handling using special representation is employed for particular types of optimization problems, whereas repair algorithms convert the infeasible individual into a feasible or less infeasible individual (Harda *et al.*, 2007). Finally, in the hybrid approach, constraint handling is tied with some other optimization approach. For example, Van Le (1995) combined fuzzy logic with evolutionary programming to handle the constraints; here; constraints are replaced by fuzzy constraints, which allow high tolerance for constraint violation. Of the five categories of constraint handling methods, penalty function and feasibility approaches have been popular for solving constrained MOO problems in chemical engineering applications; see section 5.2 for more details.

The feasibility approach can handle equality constraints via suitable transformation into inequality constraints, but this requires different values of tolerance limit for different constraints in the same problem and also for different problems. Takahama and Sakai (2006) proposed ε-constrained DE, where equality constraints are relaxed systematically. Zhang and Rangaiah (2012) proposed adaptive constraint relaxation with feasibility approach (ACRFA) for handling constraints in single objective optimization (SOO). In this approach, individuals with total constraint violation less than certain limit are temporarily considered as feasible individuals during selection for the next generation. This violation limit is changed dynamically based on the performance of the search. In this chapter, ACRFA, as proposed by Zhang and Rangaiah (2012), is modified for solving constrained MOO problems. It is implemented in the multi-objective differential evolution (MODE) algorithm and tested on two benchmark functions with equality and inequality constraints. Then, MODE with ACRFA is used to optimize two fermentation processes for two objectives; these applications involve many equality constraints arising from mass balances. The performance of ACRFA is compared with the feasibility approach alone, and discussed.

The next section of this chapter reviews recent applications of constraint handling approaches in chemical engineering. Section 5.3 describes ACRFA for constrained SOO problems, and section 5.4 presents modified ACRFA for constrained MOO problems. In section 5.5, performance of ACRFA is compared with the classical feasibility approach on two test functions. MODE with modified ACRFA is used for MOO of two fermentation processes in section 5.6. Finally, concluding remarks are made at the end of this chapter.

5.2 Constraint Handling Approaches in Chemical Engineering

Researchers have used different approaches for handling constraints in optimization problems. Selected constrained MOO studies in chemical engineering in the past decade, using stochastic algorithms with constraint handling approaches, are briefly reviewed in this section.

Li *et al.* (2003) optimized the design of a styrene reactor, where penalty function approach is used for handling constraints; they used a larger value for penalty factor to locate the global optimum precisely. Yee *et al.* (2003) used NSGA with penalty function approach to optimize the styrene reactor. Mitra *et al.* (2004) handled constraints using the feasibility approach to optimize a semi-batch epoxy polymerization process. In this study, feasibility approach is chosen for handling constraints as it does not involve any additional parameter. Tarafder *et al.* (2005) used NSGA-II with feasibility approach to optimize styrene manufacturing process for multiple objectives, and they found feasibility approach to be efficient and better than penalty function approach. Guria *et al.* (2005) have used penalty function approach for handling constraints in the optimization of reverse osmosis process for multiple objectives. Sarkar and Modak (2005) used NSGA-II with feasibility approach for MOO of fed-batch bioreactors.

Agrawal *et al.* (2006) applied NSGA-II and its jumping gene adaptations with penalty function approach for optimal design of a low-density polyethylene tubular reactor for multiple objectives. Later, Agrawal *et al.* (2007) used both penalty and feasibility approaches to handle constraints in the optimization of the same process, and found that the feasibility approach performs slightly better than penalty function approach. Sand *et al.* (2008) have used the penalty-function approach for handling constraints in batch scheduling; the penalty function approach is selected over the repair algorithm as the latter approach may introduce bias into the search. Ponsich *et al.* (2008) tried several constraint handling techniques with a genetic algorithm to optimize the design of a batch plant; these include elimination of infeasible individuals (i.e., fitness of infeasible individual = 0, which prevents selection of an infeasible individual using a roulette wheel), use of penalty term in the objective, relaxation of upper bounds for discrete variables, dominance-based tournament (similar to feasibility approach), and multi-objective strategy. Based on their results, Ponsich *et al.* (2008) concluded that elimination of infeasible individuals is most attractive when objective function calculations require less computational effort, and dominance-based tournament is better if the process model calculations require large computational time. This is mainly due to the number of (objective) function evaluations required.

Mazumder *et al.* (2010) have used NSGA-II-aJG with penalty function approach to optimize design of a liquid-solid circulating bed for continuous protein recovery, for multiple objectives. Kundu *et al.* (2012) have also used the penalty function approach to handle inequality constraints in the MOO of a counter-current moving bed chromatographic reactor. From this brief review of the selected studies it is clear that both penalty function and feasibility approaches have been used and popular for handling constraints in MOO of chemical engineering applications. Of these two, feasibility approach seems to be preferable because it does not involve any parameter and for potential computational efficiency.

5.3 Adaptive Constraint Relaxation and Feasibility Approach for SOO

Real-world optimization problems often involve both equality and inequality constraints. Although an equality constraint can be converted into an inequality constraint by a priori relaxation, feasible search space is very small in cases of problems with equality constraints, compared to complete search space and also compared to feasible search space of problems with no equality constraints. Moreover, equality constraints in chemical engineering problems arise from mass balances, mole fraction summation and/or energy balances, with terms having a wide range of magnitudes. Such equality constraints require different magnitudes of relaxation to obtain meaningful optimal solutions.

Zhang and Rangaiah (2012) introduced the concept of adaptive relaxation of constraints based on the number of feasible points obtained in each generation. First, the values of objective function and constraints are calculated for the initial population. Next, total absolute constraint violations (TACV) are calculated for each individual in the population, using:

$$\mathrm{TACV} = \sum_{i=1}^{n_e} |h_i(\mathbf{x})| + \sum_{j}^{n_i} \max[0, g_j(\mathbf{x})] \tag{5.5}$$

where h_i and g_j are the equality and inequality constraints respectively, and n_e and n_i are the number of equality and inequality constraints respectively. The median of TACV for all individuals in the initial population is chosen as the initial value for constraint relaxation (μ). Individuals are treated as temporarily feasible if their TACV is less than μ.

In the first generation, the feasibility of each individual (in differential evolution terminology, or off-spring in genetic algorithm terminology) is decided using μ value from the initial population; i.e., the individual is considered feasible if its TACV is less than μ. After that, the feasibility approach of Deb *et al.* (2002) is used to select the individuals for subsequent generation. The μ value is updated based on the number of feasible solutions obtained at the end of the first generation (see Equation 5.6), which is used to decide the feasibility of individuals in the next generation.

$$\mu_{G+1} = \mu_G \left(1 - \frac{F_F}{NP}\right) \tag{5.6}$$

Here, F_F is the fraction of feasible individuals at the end of first generation. G and NP are, respectively, the generation number and population size. The iterative procedure is repeated until the maximum number of generations.

5.4 Adaptive Relaxation of Constraints and Feasibility Approach for MOO

In the case of SOO by differential evolution (DE), selection is made between target and trial individuals. In MOO by MODE, on the other hand, nondominant sorting is employed where all target and trial individuals collectively contest for selection to the next generation. A trial individual can be temporarily feasible based on its TACV and μ, but, based on non-dominated sorting, it may not be selected for the subsequent generation. In any case, F_F can be obtained by checking the feasibility of individuals selected for subsequent generation. In the initial tests, μ value was updated using Equation 5.6 in MODE, but μ was found to decrease very fast, leading to many infeasible individuals in the population. In the case of SOO, a few feasible individuals are good enough to obtain the global solution. On the other hand, for MOO, a larger number of feasible solutions is required to obtain the Pareto-optimal front with many optimal solutions. Hence, several other relaxation schemes were tried but they all showed a fast decrease in μ value.

Finally, a different strategy is adopted for dynamically updating μ value in ACRFA for MOO problems with constraints. μ value is chosen so as to make a certain percentage of individuals selected for the next generation as infeasible. After trying μ based on 10%, 25% and 50% infeasible individuals on several test problems, a μ value corresponding to 25% infeasible individuals is found to be better. Since better individuals are selected for the next generation, μ value is expected to decrease continually; this is confirmed by results presented later.

Kukkonen and Lampinen's (2009) MODE algorithm is used for implementing and testing ACRFA (MODE-ACRFA) for solving constrained MOO problems. A flowchart of MODE-ACRFA is shown in Figure 5.1. The population of NP individuals is initialized randomly inside the bounds on decision variables. Values of objectives, constraints and TACV (according to Equation 5.5) are calculated for each individual in the initial population.

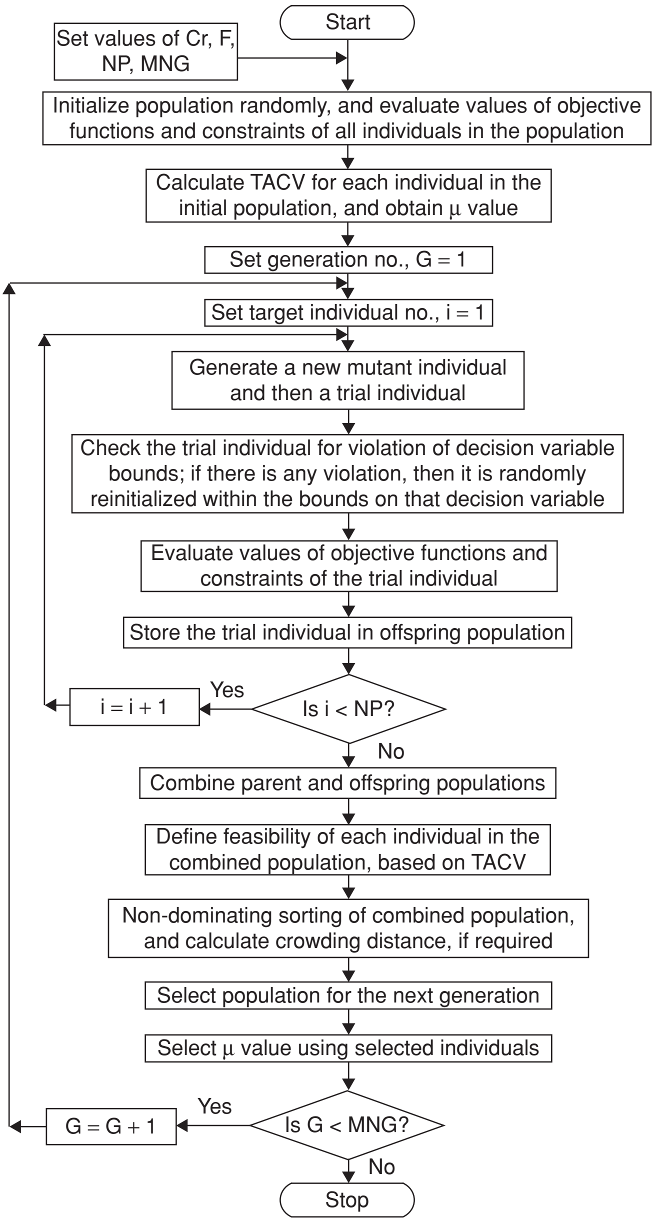

Figure 5.1 *Flowchart for MODE-ACRFA algorithm.*

Then, initial value of μ is selected such that 25% of individuals in the initial population will be temporarily infeasible based on TACV.

In each generation, a trial individual/vector for each target individual in the current/initial population is generated by mutation and crossover on three randomly selected individuals from the current/initial population. For this, DE/rand/1 mutation strategy and binomial crossover are applied according to Equations 5.7 and 5.8, respectively. See Price *et al.* (2005) for more details on these mutation and crossover operations in the differential evolution.

$$\mathbf{v}_i = \mathbf{x}_{r0} + F(\mathbf{x}_{r1} - \mathbf{x}_{r2}) \tag{5.7}$$

$$u_{i,j} = \begin{cases} v_{i,j} & \text{if } rand(0, 1) \le Cr \text{ or } j = j_{rand} \\ x_{i,j} & \text{otherwise} \end{cases} \quad j = 1, 2, \ldots, \text{no of decision variables} \tag{5.8}$$

Here, $\mathbf{v}_i$ and $\mathbf{u}_i$ are respectively mutant and trial vectors for i^{th} target individual. $\mathbf{x}_{r0}$, $\mathbf{x}_{r1}$ and $\mathbf{x}_{r2}$ are three randomly selected individuals from the current population. F and Cr are mutation rate and crossover probability, respectively. After crossover, the trial vector is tested for satisfaction of decision variable bounds; if a bound on any decision variable is violated, then it is randomly reinitialized within the bounds on that decision variable. Finally, values of objective functions, constraints and TACV of the trial individual are calculated. Thus, NP trial individuals (offspring) are generated and stored in the child population, which is later mixed with the parent population containing target individuals.

The combined population of 2NP individuals undergoes non-dominated sorting followed by crowding distance calculation. If the MOO problem has no constraints, then NP individuals are selected from the combined population based on the following definitions and steps:

1. Two individuals A and B are non-dominated to each other if A is better than B in at least one objective, and also B is better than A in at least one other objective. Thus, both these individuals are equally good. One individual is dominating another individual if it is better than the other in all objectives.
2. The number of individuals dominating each individual (n_d) is calculated. First rank is assigned to the non-dominated individuals with $n_d = 0$. This is shown as PF1 in Figure 5.2.

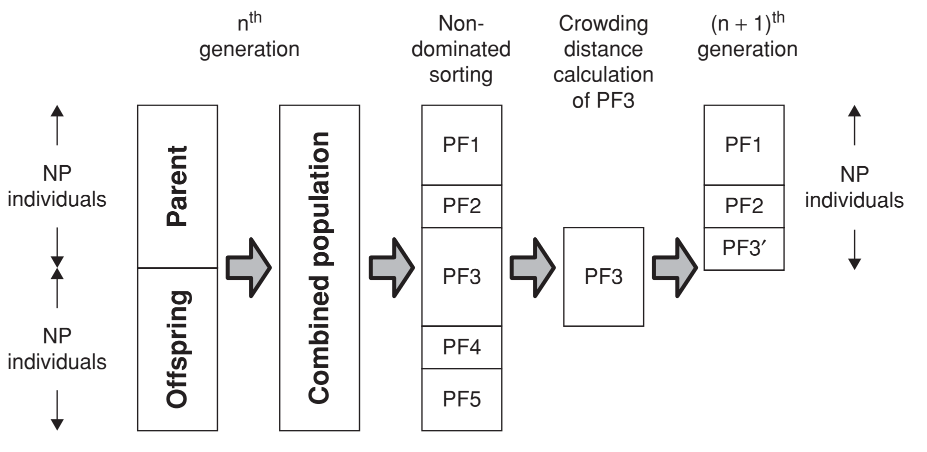

Figure 5.2 *Selection of NP individuals from the combined population of 2NP individuals using Pareto dominance and crowding distance criteria.*

3. Then, non-dominated individuals in the remainder of the combined population (i.e., excluding those with first rank) are assigned second rank (shown as PF2 in Figure 5.2). This procedure is repeated until all individuals are ranked.
4. The first/best NP individuals are selected as the population for the subsequent generation. For this, individuals are first selected based on the Pareto rank given in the above steps. When all the individuals of a Pareto front cannot be selected for the subsequent generation (e.g., PF3 in Figure 5.2), less crowded individuals (based on the crowding distance measure) are selected to complete the population size. Note that the crowding distance measures distribution of non-dominated solutions on the Pareto-optimal front by calculating Euclidean distance between two neighboring non-dominated solutions; see Deb (2001) for more details.

For constrained MOO problems, the feasibility of all individuals in the combined population is decided using the current μ value. MODE-ACRFA algorithm selects NP individuals for subsequent generation from the combined population according to steps 2–4 above, but the following definition of constrained dominance is used in step 1 (according to feasibility approach of Deb *et al.*, 2002). If any of the following conditions is true, then individual A is dominating individual B:

- Both the individuals are feasible, and individual A dominates B (as per the usual dominance definition in step a above).
- Individual A is feasible and B is infeasible.
- Both the individuals are infeasible, but individual A has smaller number of violated constraints (and lesser TACV if both have the same number of violated constraints) compared to individual B.

The TACV of selected individuals for the next generation is used to update the μ value, which is chosen so that 25% of selected individuals will be temporarily infeasible based on TACV. The new μ value is used to define the feasibility of individuals in the combined population in the next generation. The generations and stochastic search continue until the specified search termination criterion is met. Here, maximum number of generations (MNG) is the termination criterion (Figure 5.1), which is commonly used in stochastic algorithms. See Chapter 4 for performance based termination criterion for evolutionary algorithms.

5.5 Testing of MODE-ACRFA

There are many benchmark problems for testing MOO algorithms; these are with only bounds on decision variables (Zitzler *et al.*, 2000) or with both bounds on variables and inequality constraints (Coello Coello *et al.*, 2007). Interestingly, there seem to be no benchmark MOO problems with equality constraints. So, in this work, two inequality constrained MOO problems, namely, Viennet and Osyczka problems (Coello Coello *et al.*, 2007) have been modified to equality-constrained MOO problems. For this, values of different inequality constraints corresponding to the complete Pareto-optimal front have been analyzed. If an inequality constraint is active or has nearly constant value, then it is converted to an equality constraint. The modified test problems are given in Table 5.1.

Table 5.1 *Modified MOO test functions with equality constraints.*

Test problem	Decision variables	Objective functions (minimize)	Constraints
Modified Viennet	$-4 < x < 4$ $-4 < y < 4$	$F_1 = (x-2)^2/2 + (y+1)^2/13 + 3$ $F_2 = (x+y-3)^2/175 + (2y-x)^2/17 - 13$ $F_3 = (3x-2y+4)^2/8 + (x-y+1)^2/27 + 15$	$4x + y - 4 = 0$ $-x - 1 < 0$ $x - y - 2 < 0$
Modified Osyczka	$2 < x < 7$ $5 < y < 10$	$F_1 = x + y^2$ $F_2 = x^2 + y$	$x + y - 12 = 0$ $-x^2 - 10x + y^2 - 16y + 80 < 0$

The performance of MODE-ACRFA is compared with that of MODE with the feasibility approach alone (MODE-FA). For MODE-FA, each equality constraint is converted into an inequality constraint as follows.

$$h_i(\mathbf{x}) = 0 \tag{5.9}$$

$$TL - |h(\mathbf{x})| \geq 0 \tag{5.10}$$

Here, TL is the tolerance limit of constraint violation, which depends on the terms in the equality constraint (e.g., flow rates can be large whereas mole fractions are between zero and unity).

Generational distance, GD (Van Veldhuizen and Lamont, 1998) is used to compare the performance of MODE-FA and MODE-ACRFA. It is calculated between the non-dominated solutions obtained in the current/last generation and the non-dominated solutions from the known/true Pareto-optimal front as follows:

$$GD = \frac{1}{ND}\sqrt{\sum_{i=1}^{ND} d_i^2} \tag{5.11}$$

Here, ND is the number of non-dominated solutions obtained in the best front in the current generation, which can be less than or equal to the population size (i.e., NP). d_i is the Euclidean distance of each of these solutions to its nearest non-dominated solution in the known Pareto-optimal front.

Algorithm parameters used in the performance comparison for test functions/problems are: F = 0.8, Cr = 0.9, NP = 100 and MNG = 500; values of F and Cr are based on the recommendation in the literature (e.g., Chen *et al.*, 2010), while a population size of 100 is reasonable for small problems with a few decision variables and constraints. A TL value of 1.0e-6 is used for relaxing equality constraints in Table 5.1 into inequality constraints for MODE-FA. Figures 5.3(a) and 5.4(a) show the variation in GD with generations on the modified Viennet and Osyczka problems, respectively, using MODE-FA and MODE-ACRFA. The performance of both constraint-handling approaches is comparable on the modified Viennet problem. Initially, MODE-FA shows faster convergence on the modified Osyczka problem, but performance of both approaches is comparable after 200 generations (Figure 5.4a). Moreover, the final Pareto-optimal fronts obtained for both the problems using ACRFA and FA are very close to the true Pareto-optimal fronts, as shown in Figures 5.3 and 5.4.

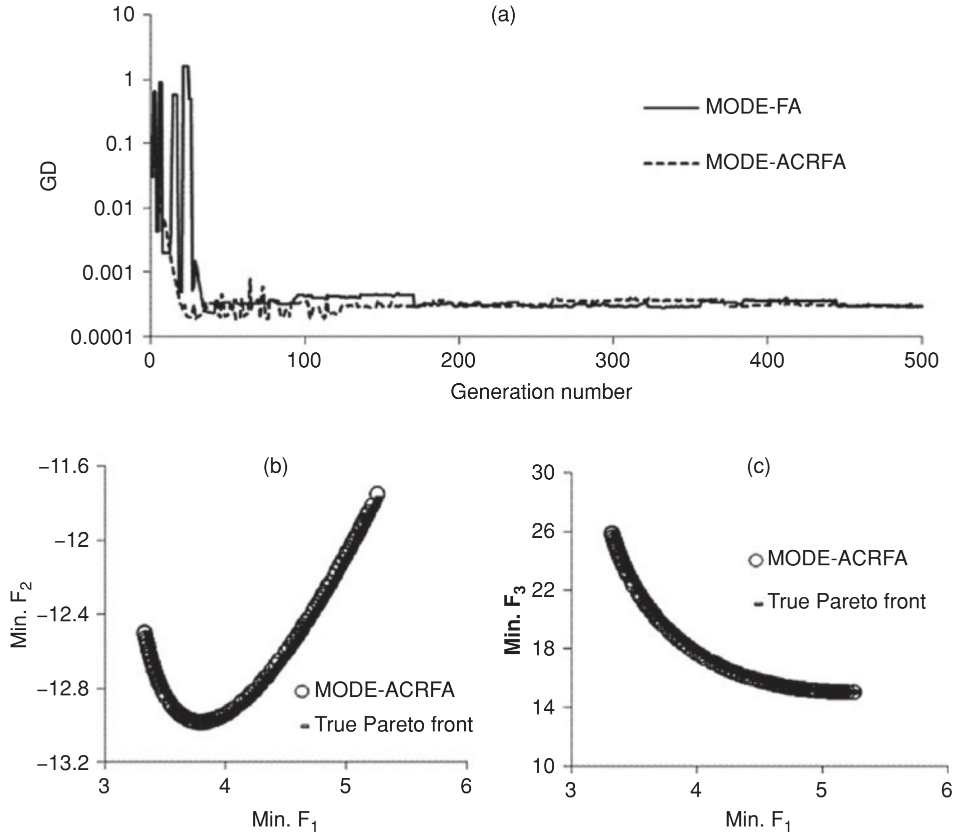

Figure 5.3 *Performance of MODE-FA and MODE-ACRFA on the modified Viennet problem.*

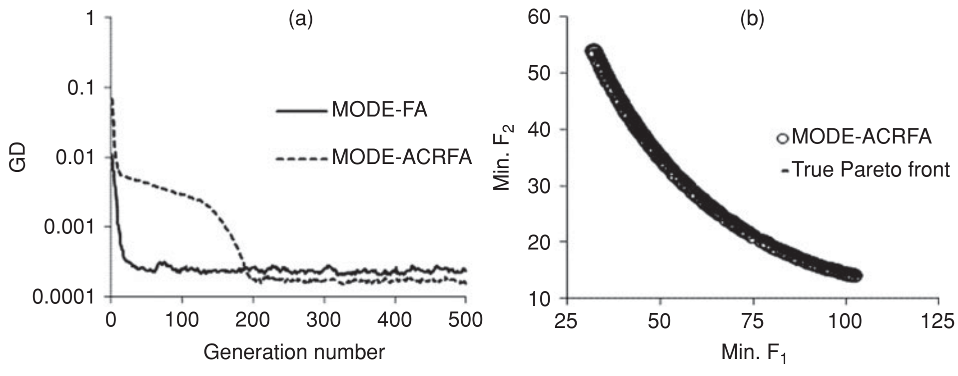

Figure 5.4 *Performance of MODE-FA and MODE-ACRFA on the modified Osyczka problem.*

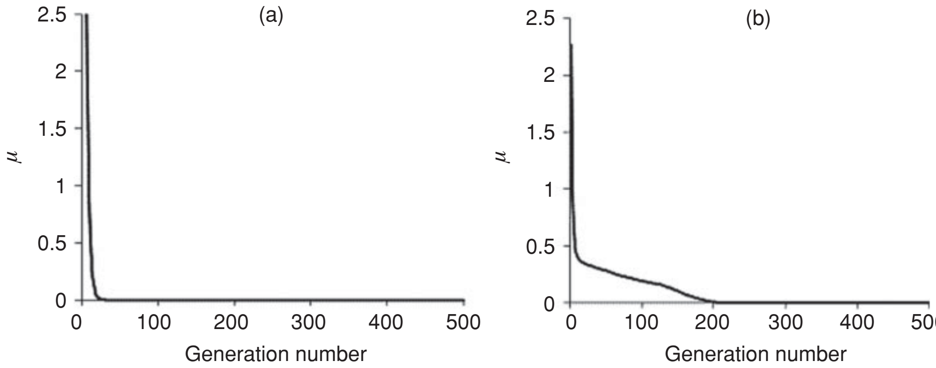

Figure 5.5 *Variation in μ with generations in MODE-ACRFA on: (a) Viennet problem, and (b) Osyczka problem.*

Figure 5.5 shows the variation in μ with generations on the Viennet and Osyczka problems using MODE-ACRFA; these follow the general trend of GD with generations in Figures 5.3(a) and 5.4(a). As expected, μ decreases with generations because better individuals (in terms of feasibility and objective values) are selected for the next generation.

5.6 Multi-Objective Optimization of the Fermentation Process

Ethanol is widely used as a chemical and biofuel. Bioethanol production from sustainable feedstocks is one of the possible alternatives to fossil fuel. Its production using first-generation feedstocks (e.g., glucose) is well established, while bioethanol production using second generation feedstocks (e.g., starch and cellulose) is in the development phase. In this section, operation of a fermentation process integrated with cell recycling and a fermentation process integrated with cell recycling and inter-stage extraction is optimized for multiple objectives by both MODE-FA and MODE-ACRFA. Both these applications involve equality constraints.

5.6.1 Three-Stage Fermentation Process Integrated with Cell Recycling

Wang and Lin (2010) have studied a three-stage continuous fermentation process integrated with cell recycling, where each stage has a fermentor and a cell separator to separate the cell mass and recycle it back to the fermentor, for ethanol production from glucose. A schematic diagram of this fermentation process integrated with cell recycling is shown in Figure 5.6.

Equations 12–14 present steady-state material balances for cell mass, glucose and ethanol respectively, around the k^{th} stage of continuous fermentation process. The used kinetic model is given by Equations 5.15 and 5.16. Equations for all the three stages including kinetic parameter values are available in one Excel file on the web site for this book.

$$D\,[b_{k-1}x_{k-1} - b_k x_k] + \mu_k x_k = 0 \tag{5.12}$$

$$D\left[s_{f,k} + s_{k-1} - s_k\right] - \frac{q_{p,k}}{Y_{p/s}} x_k = 0 \tag{5.13}$$

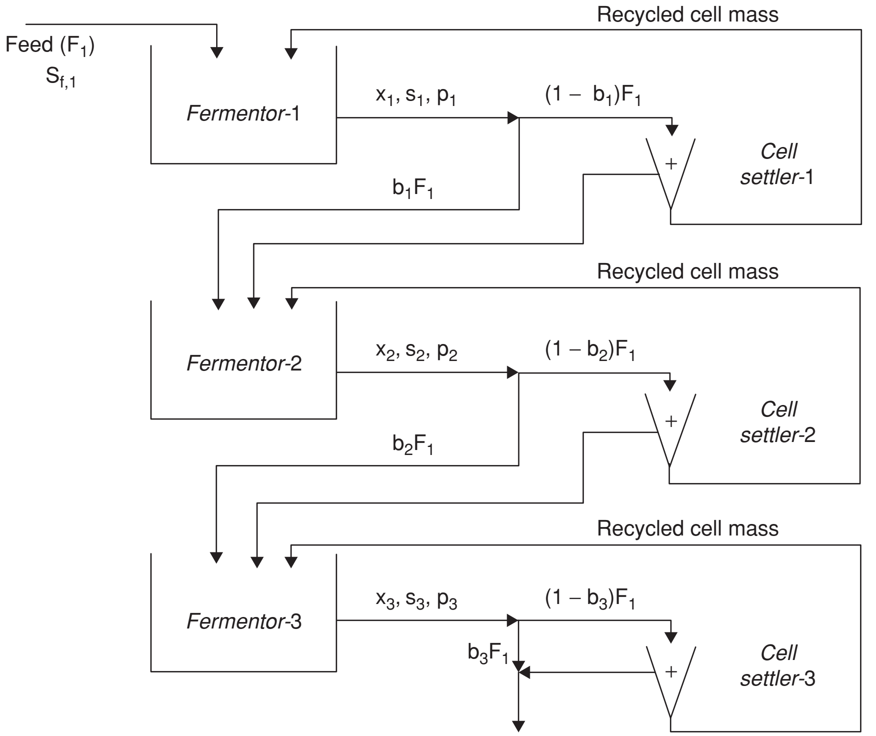

Figure 5.6 *Schematic diagram of a three-stage continuous fermentation process integrated with cell recycling.*

$$D\left[p_{k-1} - p_k\right] + q_{p,k}x_k = 0 \tag{5.14}$$

$$\mu_k = \left(\frac{\mu_m s_k}{K_s + s_k + s_k^2/K_{sI}}\right)\left(\frac{K_p}{K_p + p_k + p_k^2/K_{pI}}\right) \tag{5.15}$$

$$q_{p,k} = \left(\frac{\nu_m s_k}{K_s' + s_k + s_k^2/K_{sI}'}\right)\left(\frac{K_p'}{K_p' + p_k + p_k^2/K_{pI}'}\right) \tag{5.16}$$

Here, D ($= F_1/V$) is the dilution rate, F_1 is the feed flow rate to the first stage, and V is the volume of each fermentor. x_k, s_k and p_k are respectively cell mass, glucose and ethanol concentrations in k^{th} stage; b_k is the bleed ratio for k^{th} stage. $s_{f,k}$ is glucose concentration in the feed to k^{th} stage; as feed is entering only into the firststage, $s_{f,2} = 0$ and $s_{f,3} = 0$ for the second and third stages. Further, for the first stage, b_{k-1}, x_{k-1}, s_{k-1} and p_{k-1} are all zero. Kinetic parameter values used in Equations 5.12–5.16 are listed in Table 5.2.

To optimize the fermentation process, ethanol productivity and glucose conversion are used as two objectives, which ensure efficient utilization of production capacity and glucose respectively. The MOO problem for the three-stage continuous fermentation process integrated with cell recycling is summarized in Table 5.3. Decision variables for this optimization are dilution rate (D), glucose concentration in feed ($s_{f,1}$) and cell mass recycling

Table 5.2 *Kinetic parameters and their values for the continuous fermentation process integrated with cell recycling (Wang and Sheu, 2000).*

Kinetic parameter	Estimated value	Kinetic parameter	Estimated value
μ_m	0.9819	K_p	27.9036
ν_m	2.3507	K'_p	252.306
K_s	2.3349	K_{pI}	41.2979
K'_s	7.3097	K'_{pI}	15.2430
K_{sI}	213.5899	$Y_{p/s}$	0.4721
K'_{sI}	5759.105		

for different stages (i.e., bleed ratios, b_1, b_2 and b_3). Physical constraints are positive values of productivity and glucose conversion for each stage. Residual glucose after the third stage and total glucose supplied per unit volume of all fermentors in the feed are additional constraints in the optimization problem (Wang and Lin, 2010). The model Equations 5.12 to 5.16 for each stage are the equality constraints in the MOO problem. Of these, Equations 5.15 and 5.16 can be substituted in Equations 5.12 to 5.14. Then, there will be three equality constraints for each stage or nine equality constraints for the three-stage fermentation process.

Wang and Lin (2010) have solved the MOO problem in Table 5.3 using the fuzzy goal attainment method, which requires preference intervals for objectives and constraints. Finally, it is solved as a SOO problem using hybrid differential evolution (HDE). The adaptive penalty function approach has been used for constraint handling in HDE. The same optimization approach (i.e., HDE with an adaptive penalty function approach) is also used to solve the MOO problem of extractive fermentation process (section 5.6.2). In this work, MOO problem (Table 5.3) has been solved by three different strategies, all using

Table 5.3 *MOO problem formulation for the three-stage continuous fermentation process integrated with cell recycling.*

Objective functions	Max. ethanol productivity	$\frac{D}{3}p_3$ [kg/(m^3.h)]
	Max. overall glucose conversion	$1 - \frac{s_3}{s_{f,1}}$
Decision variables	Dilution rate	$3.5 \leq D \leq 4$ [1/h]
	Glucose concentration in feed	$60 \leq s_{f,1} \leq 65$ [kg/m^3]
	Bleed ratio for each stage	$0.1 \leq b_1 = b_2 = b_3 \leq 0.2$
Constraints	Productivity for each stage	$D[p_k - p_{k-1}] \geq 0$ for k = 1, 2, 3 [kg/(m^3.h)]
	Glucose conversion for each stage	$1 - \frac{s_k}{s_{f_k}+s_{k-1}} \geq 0$ for k = 1, 2, 3
	Residual glucose after 3rd stage	$0.1 \leq s_3$; and $s_3 \leq 0.5$ [kg/m^3]
	Total glucose supplied per unit volume of all fermentors	$10 \leq s_T$; and $s_T \leq 180$; $s_T \equiv \frac{Ds_{f,1}}{3}$ [kg/(m^3.h)]
	Model for the process	Equations 5.12 to 5.16 for each stage

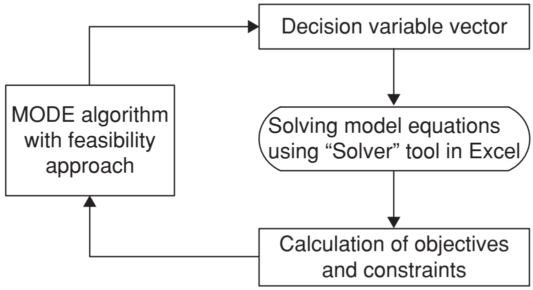

Figure 5.7 Flowchart for calculation of objective functions and constraints using "Solver" tool in Excel for solving process model equations.

MODE. Each strategy differs in the handling of constraints, as described below. The present approach provides many Pareto-optimal solutions for better understanding and selection of one of them.

(A) MODE-Solver and FA: In this approach, the MODE algorithm has been used to generate the vector of three decision variables (i.e., D, S_f, and b). In order to calculate objectives and constraints, material balance equations 5.12–5.14 for each stage have to be solved; Solver tool in Excel is used to solve these equations (see Figure 5.7). The feasibility approach is used to handle inequality constraints in the optimization problem (a total of ten inequality constraints in Table 5.3 excluding the model equations). This strategy is used to illustrate the use of the sequential solution of optimization problem and equality constraints (i.e., model equations), and to obtain the Pareto-optimal solutions for comparison.

(B) MODE-FA: In this approach, material balance equations 5.12–5.14 for each stage are converted into inequality constraints; conversion of each equality constraint to an inequality constraint is based on Equations 5.9 and 5.10 and using the same value of TL. Finally, the reformulated MOO problem has 19 inequality constraints (ten inequality constraints in Table 5.3, and nine inequality constraints from material balances for each stage). For this and the next strategy, additional decision variables are cell mass, glucose and ethanol concentrations for each stage. These variables with their bounds are presented in Table 5.4; non-dominated solutions obtained, using strategy A, are used to choose suitable bounds on the additional decision variables. Thus, the number of decision variables in this and next strategy is 12.

(C) MODE-ACRFA: This approach can handle equality constraints without any conversion. It has nine equality and ten inequality constraints. Decision variables are the

Table 5.4 *Additional decision variables and their bounds for optimization strategies B and C.*

Decision variable	x_1	x_2	x_3	s_1	s_2	s_3	p_1	p_2	p_3
Lower bound	40	80	90	10	0	0.1	10	20	20
Upper bound	70	110	110	30	10	0.5	30	40	40

Table 5.5 *MODE algorithm parameter values used in MOO of fermentation processes.*

Algorithm parameter	Strategy A: MODE-Solver with FA	Strategy B: MODE-FA	Strategy C: MODE-ACRFA
F	0.9	0.9	0.9
Cr	0.9	0.9	0.9
NP	100	465	465
MNG	100	5000	5000

same as those in MODE-FA. Optimization problem and equality constraints are solved simultaneously in both MODE-FA and MODE-ACRFA. However, solution of equality constraints in MODE-FA is not exact due to relaxation by TL, and so its optimization results can differ from the other two strategies.

MODE parameters used in this optimization study are given in Table 5.5. The F value is tuned through preliminary experimentation, whereas the Cr value is based on the recommendation in the literature (see Chen *et al.*, 2010). The population size of 100 is used in solution strategy A, while the population size in solution strategies B and C is 15 times the sum of the number of decision variables and constraints. MNG used for different strategies is based on preliminary experimentation.

Figure 5.8(a) shows the Pareto-optimal front obtained for the three-stage continuous fermentation process integrated with cell recycling using strategy A. As expected, ethanol productivity is conflicting with glucose conversion. The obtained Pareto-optimal front is well distributed, and dilution rate is mainly contributing to the variations in the objective functions. Glucose concentration in the feed and bleed ratios are nearly constant, and they are near to their upper (i.e., 65) and lower (i.e., 0.1) bounds respectively. For brevity, bleed ratios are not shown in Figure 5.8. The Pareto-optimal front obtained in Figure 5.8(a) is nearly linear in shape. In the operation optimization considered, production capacity is sufficiently large to convert glucose completely for any dilution rate in the range 3.5 to 4; hence, glucose concentration in the feed is always near to its upper limit (see Figure 5.8c). A further, increase in dilution rate increases ethanol productivity as a larger amount of glucose enters into the fermentor although glucose conversion decreases due to lower residence time. Both objectives are linearly dependent on dilution rate because the quantities (i.e., dilution rate, ethanol concentration in the product stream, glucose concentration in feed and residual glucose) involved in the objectives are directly related to the dilution rate (see Table 5.3).

Figure 5.8(a) also shows the Pareto-optimal front obtained for the same continuous fermentation process using MODE-FA. These optimization results are obtained using TL of 3.0; MODE-FA did not give any feasible solution with a TL of 1.0 or smaller. The non-dominated solutions in Figure 5.8(a) have average absolute constraint violations (AACV) of 2.15. Here, variation in ethanol productivity is smaller compared to the Pareto-optimal front obtained using strategy A (Figure 5.8a). Figures 5.8(b) and 5.8(c) show, respectively, the variations in dilution rate and glucose concentration in the feed with ethanol productivity. Bleed ratio is constant near to 0.1, and so this is not shown in Figure 5.8. Variations in the remaining decision variables for strategies B and C (in Table 5.4) are also not presented as

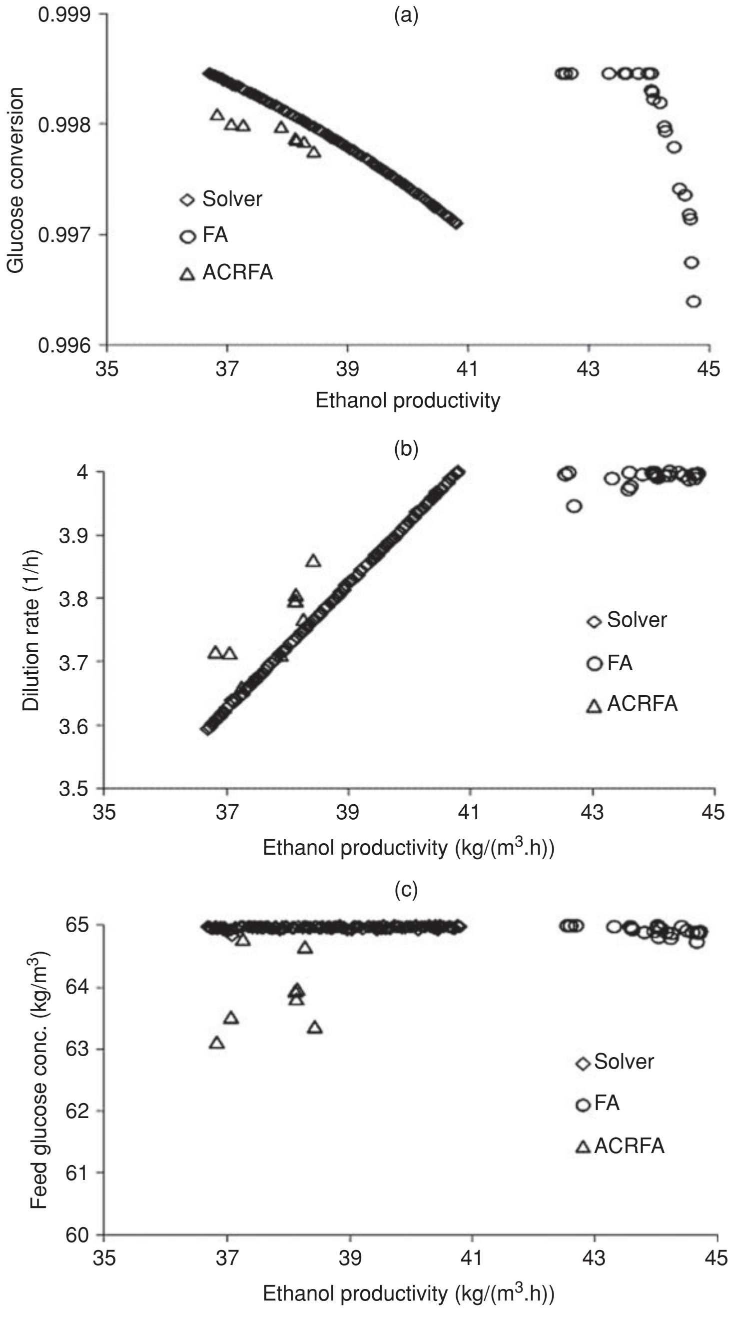

Figure 5.8 *Selected optimization results for a three-stage continuous fermentation process integrated with cell recycling, using strategies A (Solver), B (FA), and C (ACRFA).*

these are not essential for performance comparison. Pareto-optimal front obtained for the three-stage continuous fermentation process integrated with cell recycling using MODE-ACRFA is also shown in Figure 5.8(a). Here, both objectives are varying in narrow ranges compared to the other two; AACV for all non-dominated solutions obtained by MODE-ACRFA is 0.013, which is much smaller than that by MODE-FA.

Figure 5.8(a) can be used for comparing the non-dominated solutions obtained for the three-stage continuous fermentation process integrated with cell recycling using three different optimization strategies. In this comparison, Pareto-optimal front obtained by MODE-Solver with FA can be considered as the correct front. It can be seen that non-dominated solutions obtained using MODE-FA are significantly far from the correct Pareto-optimal front; also they have high value of AACV (= 2.15), and so they are not the optimal solutions satisfying all constraints. On the other hand, non-dominated solutions obtained by MODE-ACRFA are close to the correct Pareto-optimal front, and they have a much lower value of AACV (= 0.013), which is acceptable in engineering applications.

5.6.2 Three-Stage Fermentation Process Integrated with Cell Recycling and Extraction

Chen and Wang (2010) have studied a three-stage fermentation process integrated with cell recycling and inter-stage extraction using a mixture of glucose and xylose as feedstocks (referred to as simply extractive fermentation from now on). Figure 5.9 shows a schematic diagram of this fermentation process. Ethanol concentration inhibits conversion of glucose

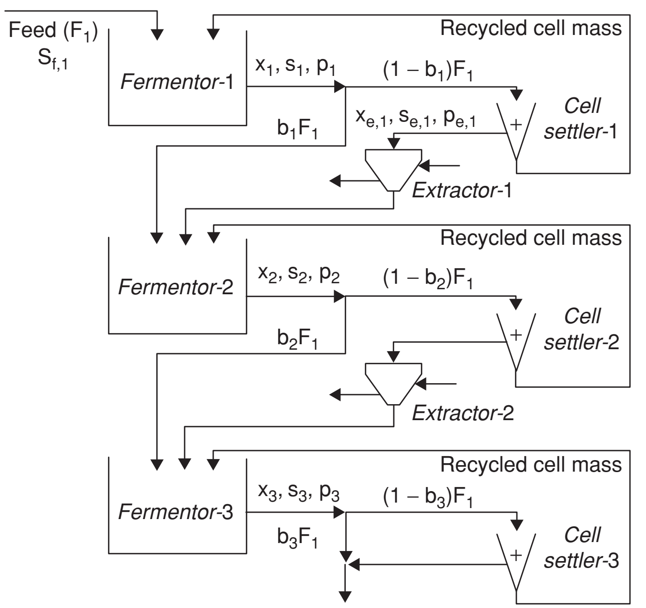

Figure 5.9 *Schematic diagram of a three-stage fermentation process integrated with cell recycling and extraction.*

and xylose to ethanol in the fermentor, which results in lower ethanol productivity and yield. To avoid this, ethanol can be removed continuously from the fermentor, for example using extraction. In the present study, three fermentors are placed in series, with feed entering into the first fermentor only. Part of the mother liquor from a fermentor goes directly to the next fermentor while the remainder goes through a cell separator and an extractor. A cell separator is used after each fermentor to separate the cell mass and recycle it back to the fermentor, whereas an extractor is used to extract ethanol using an organic solvent. After extraction of ethanol, mother liquor goes to the next fermentor. An extractor is not necessary in the last/third stage of the fermentation process (see Figure 5.9).

The mathematical model of the three-stage extractive fermentation process is taken from Chen and Wang (2010). Equations 5.17–5.20 present steady-state mass balances for cell mass, glucose, xylose and ethanol around k^{th} stage, respectively. Equations for all the three stages including kinetic parameter values are available in the Excel file on the web site for this book.

$$D\left[b_{k-1} + (1 - b_{k-1})\,\zeta_x\right] x_{k-1} - D\left[b_k + (1 - b_k)\,\zeta_x\right] x_k + r_{x,k} = 0 \tag{5.17}$$

$$D\lambda s_{f,k} + D\left[b_{k-1} + (1 - b_{k-1})\,\zeta_s\right] s_{g,k-1} - D[b_k + (1 - b_k)\,\zeta_s] s_{g,k} - r_{sg,k} = 0 \tag{5.18}$$

$$D(1 - \lambda) s_{f,k} + D\left[b_{k-1} + (1 - b_{k-1})\,\zeta_s\right] s_{x,k-1} - D[b_k + (1 - b_k)\,\zeta_s] s_{x,k} - r_{sx,k} = 0 \tag{5.19}$$

$$D\left[b_{k-1} + (1 - b_{k-1})\,\frac{\zeta_p}{1 + E_{k-1}}\right] p_{k-1} - D\left[b_k + (1 - b_k)\,\zeta_p\right] p_k + r_{p,k} = 0 \tag{5.20}$$

In the above equations, D is the dilution rate. x_k, $s_{g,k}$, $s_{x,k}$ and p_k are respectively cell mass, glucose, xylose and ethanol concentration (kg/m^3) in k^{th} stage fermentor. b_k is the bleed ratio for k^{th} stage, and $s_{f,k}$ is the substrate concentration in feed entering k^{th} stage. λ is the mass fraction of glucose in substrate (and the remaining is xylose). ζ_x, ζ_s and ζ_p are cell discard factors (e.g., $x_{e,1}/x_1 = 0.01$), substrate condensed factors (e.g., $s_{e,1}/s_1 = 1.01$) and ethanol condensed factors (e.g., $p_{e,1}/p_1 = 1.01$) respectively (see Figure 5.9); these factors define relative concentrations of cell mass, substrate and ethanol in mother liquor after cell separation compared to those after the fermentor. E_k is the extraction efficiency for k^{th} stage. Here, feed is entering only into the first fermentor, and so values of $s_{f,2} = 0$ and $s_{f,3} = 0$ for second and third stages respectively. Further, for the first stage, b_{k-1}, x_{k-1}, $s_{g,k-1}$, $s_{x,k-1}$, p_{k-1} and E_{k-1} are also zero.

The rate expressions for cell mass growth ($r_{x,k}$), glucose consumption ($r_{sg,k}$), xylose conversion ($r_{sx,k}$) and ethanol production ($r_{p,k}$) are as follows.

$$r_{x,k} = \mu_{mix,k} x_k \tag{5.21}$$

$$r_{sg,k} = \frac{1}{Y_{p/sg}} \nu_{g,k} x_k \tag{5.22}$$

$$r_{sx,k} = \frac{1}{Y_{p/sx}} \nu_{x,k} x_k \tag{5.23}$$

$$r_{p,k} = \left(\nu_{g,k} + \nu_{x,k}\right) x_k \tag{5.24}$$

Here, μ_{mix} is the specific cell growth rate for the yeast 1400 (pLNH33) on glucose-xylose mixture. For this yeast, ν_g and ν_x are the specific production rates of glucose and xylose, respectively. μ_{mix}, ν_g and ν_x are defined as follows.

$$\mu_{g,k} = \frac{\mu_{mg} s_{g,k}}{K_g + s_{g,k} + s_{g,k}^2/K_{ig}} \left\{1 - \left(\frac{p_k}{p_{mg}}\right)^{\Phi_g}\right\} \tag{5.25}$$

$$\mu_{x,k} = \frac{\mu_{mx} s_{x,k}}{K_x + s_{x,k} + s_{x,k}^2/K_{ix}} \left\{1 - \left(\frac{p_k}{p_{mx}}\right)^{\Phi_x}\right\} \tag{5.26}$$

$$\mu_{mix} = \frac{s_{g,k}}{s_{g,k} + s_{x,k}} \mu_{g,k} + \frac{s_{x,k}}{s_{g,k} + s_{x,k}} \mu_{x,k} \tag{5.27}$$

$$\nu_{g,k} = \frac{\nu_{mg} s_{g,k}}{K'_g + s_{g,k} + s_{g,k}^2/K'_{ig}} \left\{1 - \left(\frac{p_k}{p'_{mg}}\right)^{\varphi_g}\right\} \tag{5.28}$$

$$\nu_{x,k} = \frac{\nu_{mx} s_{x,k}}{K'_x + s_{x,k} + s_{x,k}^2/K'_{ix}} \left\{1 - \left(\frac{p_k}{p'_{mx}}\right)^{\varphi_x}\right\} \tag{5.29}$$

The kinetic parameters in Equations 5.21–5.29 are taken from Krishnan *et al.* (1999), and are reported in Table 5.6.

The MOO problem formulation for the three-stage extractive fermentation process is given in Table 5.7. In this case, ethanol productivity and xylose conversion are considered as objectives. Glucose conversion is not used as an objective because it is always higher than xylose conversion; it is used as an additional constraint in the optimization problem. Dilution rate and substrate concentration in the feed are the decision variables. Bleed ratios for different stages are not considered as decision variables, as low values are optimal, based on section 5.6.1; so, bleed ratio for each of the stages is fixed at 0.2. Here, positive values of ethanol productivity of each stage, glucose and xylose conversions in each stage are physical constraints. Other constraints are total sugar supply ($s_T < 180$) and limits on

Table 5.6 *Kinetic parameters and their values for extractive fermentation process (Krishnan* et al.*, 1999).*

Kinetic parameters	Estimated values
μ_{mg}, μ_{mx} (h^{-1})	0.662, 0.190
ν_{mg}, ν_{mx} (h^{-1})	2.005, 0.250
K_g, K_x (kg/m^3)	0.565, 3.4
K_{ig}, K_{ix} (kg/m^3)	283.7, 18.1
K'_g, K'_x (kg/m^3)	1.342, 3.4
K'_{ig}, K'_{ix} (kg/m^3)	4890, 81.3
p_{mg}, p_{mx} (kg/m^3)	95.4, 59.04
p'_{mg}, p'_{mx} (kg/m^3)	103.03, 60.2
Φ_g, Φ_x	1.29, 1.036
φ_g, φ_x	1.42, 0.608
$Y_{p/sg}$, $Y_{p/sx}$ (kg/kg)	0.47, 0.40

Table 5.7 *MOO problem formulation for the extractive fermentation process.*

Objective function	Max. ethanol productivity	$\frac{D}{3}[b_3 + (1 - b_3)\zeta_p]p_3 + \sum_{k=1}^{2}(1 - b_k)\frac{\zeta_p E}{(1+E)}p_k$ [kg/(m^3.h)]
	Max. overall xylose conversion	$1 - \frac{[b_3+(1-b_3)\zeta_s]s_{x,3}}{(1-\lambda)s_{f,1}}$
Decision variables	Dilution rate	$0.3 \le D \le 0.8$ [1/h]
	Substrate conc. in feed	$90 \le s_{f,1} \le 95$ [kg/m^3]
Constraints	Productivity in each stage	$D\left[\left\{b_k + (1 - b_k)\,\zeta_p\right\}p_k - \left\{b_{k-1} + \frac{1-b_{k-1}}{1+E_{k-1}}\zeta_p\right\}p_{k-1}\right] \ge 0$ for k = 1, 2, 3 [kg/(m^3.h)]
	Glucose conversion in each stage	$1 - \frac{\{b_k+(1-b_k)\zeta_s\}s_{g,k}}{\lambda s_{f,k}+\left\{b_{k-1}+\left(1-b_{k-1}\right)\zeta_s\right\}s_{g,k-1}} \ge 0$ for k = 1, 2, 3
	Xylose conversion in each stage	$1 - \frac{\{b_k+(1-b_k)\zeta_s\}s_{x,k}}{(1-\lambda)s_{f,k}+\left\{b_{k-1}+\left(1-b_{k-1}\right)\zeta_s\right\}s_{x,k-1}} \ge 0$ for k = 1, 2, 3
	Residual glucose	$s_{g,3} \le 0.5$ [kg/m^3]
	Residual xylose	$s_{x,3} \le 1$ [kg/m^3]
	Total glucose supplied per unit volume	$s_T \equiv \frac{Ds_{f,1}}{3} \le 180$ [kg/(m^3.h)]
	Glucose conversion overall	$1 - \frac{[b_3+(1-b_3)\zeta_s]s_{g,3}}{\lambda s_{f,1}} > 0.99$
	Model for the process	Equations 5.17 to 5.29 for each stage

Table 5.8 *Additional decision variables and their bounds for optimization strategies B and C.*

Decision variable	x_1	x_2	x_3	s_{g1}	s_{g2}	s_{g3}	s_{x1}	s_{x2}	s_{x3}	p_1	p_2	p_3
Lower bound	0	20	50	0	0	0	20	0	0	20	10	0
Upper bound	20	60	70	10	1	10	40	20	1	40	30	20

the residual glucose and xylose concentrations ($s_{g,3} < 0.5$ and $s_{x,3} < 1$) in the mother liquor from the third fermentor (Chen and Wang, 2010). The model Equations 5.17 to 5.29 for each stage are the equality constraints in the MOO problem. Of these, Equations 5.21 to 5.29 can be substituted in Equations 5.17 to 5.20. Then, there will be four equality constraints for each stage or 12 equality constraints for the three-stage extractive fermentation process.

The MOO problem in Table 5.7 is solved using three different strategies, described in section 5.6.1. The problem for strategy A (using Solver and FA) has two decision variables and 13 inequality constraints. Reformulation of the problem for MODE-FA has 12 additional inequality constraints arising from material balances around each and every stage (in total, 25 inequality constraints). Problem for MODE-ACRFA has 13 inequality and 12 equality constraints. Moreover, the problem for both MODE-FA and MODE-ACRFA has 12 additional decision variables (i.e., cell mass, glucose, xylose and ethanol concentrations for each of the three stages); these variables and their bounds are listed in Table 5.8. Very wide bounds for additional decision variables (e.g., 0 to 1000) will result in slow convergence of the algorithm; hence, non-dominated solutions obtained using strategy A are used to choose the bounds on the additional decision variables.

The feed contains 65% glucose and 35% xylose, and extraction efficiency for each stage is 6.93, which is equivalent to 87.4% of ethanol removal from the mother liquor (Chen and Wang, 2010). The MODE algorithm parameters used in the optimization of extractive fermentation process are same as those in Table 5.5, except the value of NP for strategies B and C is 585 (i.e., 15 times the number of decision variables and constraints).

Figure 5.10(a) shows the Pareto-optimal front obtained for the three-stage extractive fermentation process using optimization strategy A (i.e., Solver for solving equality constraints/model equations with FA for inequality constraints; see section 5.6.1). The obtained Pareto-optimal front can be divided into two parts: (i) improvement in ethanol productivity from 5.4 to 5.8 kg/(m3.h) with a small decrease in xylose conversion, and (ii) a linear change between ethanol productivity and xylose conversion ($\sim$ 0.985–0.97). In the first part, the improvement in ethanol productivity, is mainly due to fast change in substrate concentration in feed, while dilution rate is mainly affecting the objectives in the second part (see Figures 5.10a–c). For a fixed production capacity, an increase in substrate concentration in the feed produces more ethanol but it does not affect residence time in the fermentor. Hence, an increase in ethanol productivity is relatively faster compared to decrease in xylose conversion (see the first part of the Pareto-optimal front in Figure 5.10a). Increase in dilution rate also increases ethanol productivity as a larger amount of glucose enters into fermentors, but substrate conversion decreases relatively faster with an increase in dilution rate due to lower residence time (see the second part of the Pareto-optimal front obtained in Figure 5.10a). In conclusion, a relatively fast increase in ethanol productivity is

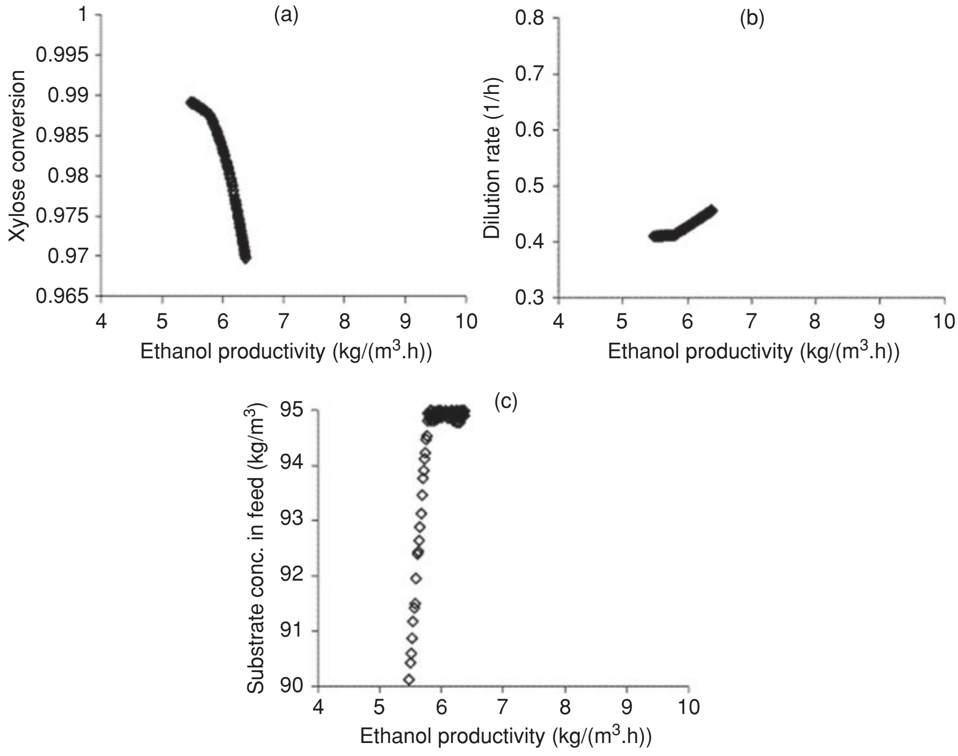

Figure 5.10 *Selected optimization results for the 3-stage extractive fermentation process using optimization strategy A (Solver and FA).*

achieved initially by an increase in substrate concentration in the feed, until substrate concentration reached availability limit. In the present operation optimization case, the ethanol production facility is sufficient to convert feed, at its maximum available concentration (i.e., 95 kg/m^3), into product, and keeps the unreacted substrate in the product stream below the required limit.

Figure 5.11(a) shows the Pareto-optimal front obtained for the three-stage extractive fermentation process using MODE-FA. These non-dominated solutions are obtained using TL of 1.0; MODE-FA is not able to give any feasible solution with a smaller value of TL. The non-dominated solutions in Figure 5.11(a) have an AACV of 0.608. Variations in objectives can be visually correlated to the variation in dilution rate with ethanol productivity (Figure 5.11b), while substrate concentration in feed is scattered between its lower and upper bounds (Figure 5.11c).

The Pareto-optimal front obtained by MODE-ACRFA is shown in Figure 5.11(d). Here, both objectives are varying in relatively narrow ranges compared to the Pareto-optimal front obtained using the other two strategies. AACV for all non-dominated solutions obtained using MODE-ACRFA is 0.022, which is acceptable for engineering applications. Values and trends in the Pareto-optimal front and decision variables in Figures 5.11(d) to (f) are similar to those obtained by strategy A (Figure 5.10).

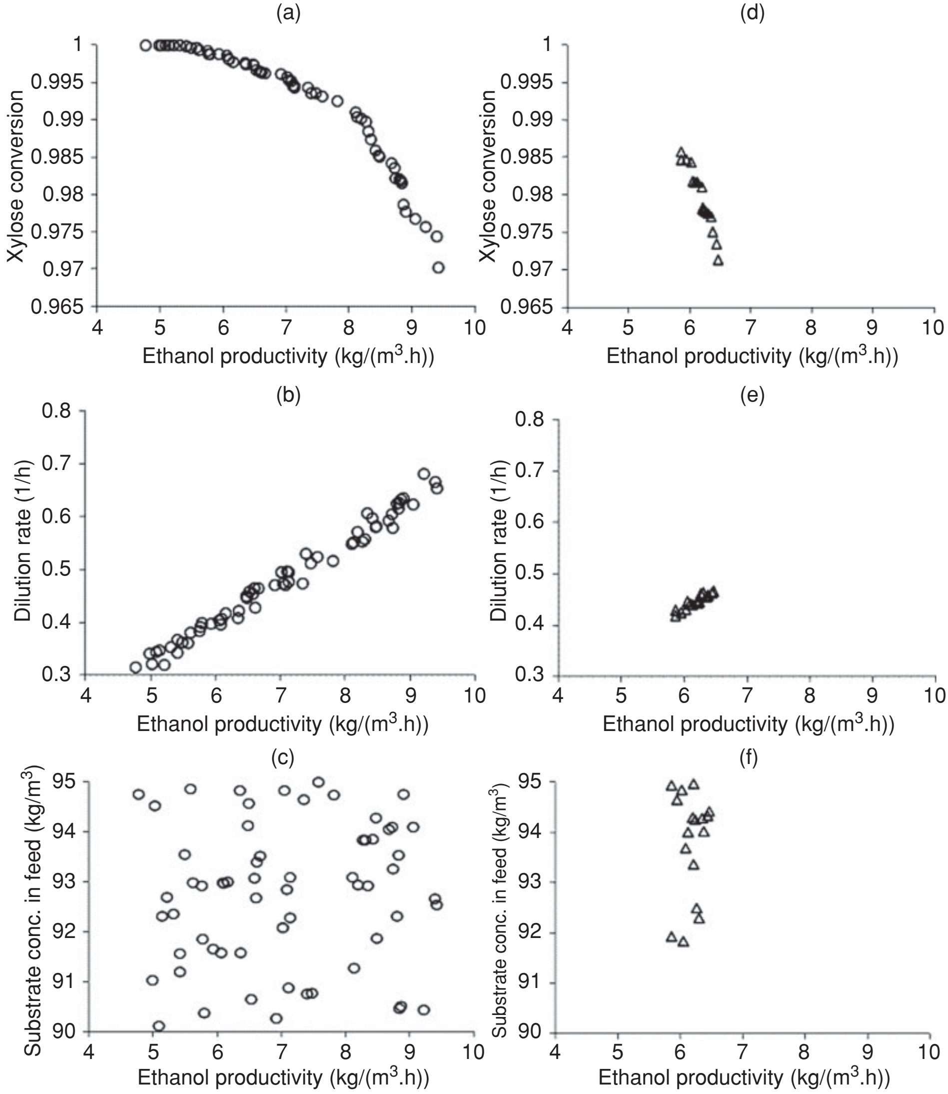

Figure 5.11 *Selected optimization results for the three-stage extractive fermentation process using MODE-FA (plots a, b and c in the left column), and using MODE-ACRFA (plots d, e and f in the right column).*

Finally, Figure 5.12 compares the Pareto-optimal fronts obtained for extractive fermentation process using the three different optimization strategies. Pareto-optimal front obtained by strategy A (i.e., MODE-Solver-FA) can be considered as the correct solution to this problem. It can be seen that MODE-FA (Strategy B) gives wide ranges of both objectives, but these non-dominated solutions have a large value of AACV, and so they are incorrect and unacceptable. The non-dominated solutions obtained by MODE-ACRFA (Strategy C) are

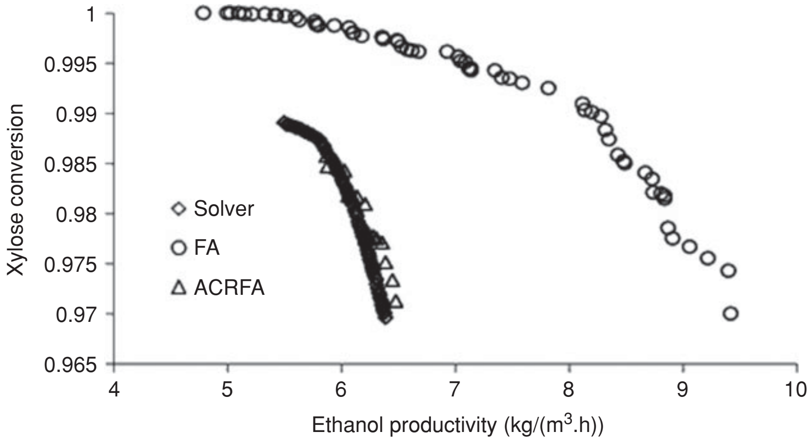

Figure 5.12 *Comparison of the Pareto-optimal fronts obtained for the three-stage fermentation process integrated with cell recycling and inter-stage extraction, using three different optimization strategies.*

closer to the correct Pareto-optimal front, and cover most part of the correct Pareto-optimal front except a small part corresponding to higher xylose conversion.

5.6.3 General Discussion

It is clear from the results in sections 5.6.1 and 5.6.2 that optimal non-dominated solutions obtained by MODE-Solver and FA (Strategy A) are better; they satisfy equality constraints almost exactly and so can be considered to be accurate. Non-dominated solutions obtained by MODE-FA (strategy B) are affected by the TL used; their validity is questionable due to constraint violations (i.e., the larger value of AACV). MODE-ACRFA gives optimal solutions which satisfy the equality constraints; they are comparable to those obtained by strategy A, although their range is narrow.

The approximate time required for solving the MOO problem for the continuous fermentation process using strategies A, B and C is respectively 1, 8 and 3 hours on an Intel® Core™2 Duo Processor (CPU 2.8 & 2.8 GHZ and RAM 4 GB). Mflops (million floating point operations per second) on this computer is 537 for the LINPACK benchmark program for a matrix of order 500 (http://www.netlib.org/benchmark/linpackjava/). Optimization of the extractive fermentation process requires around 2, 12 and 4 hours by strategies A, B and C respectively, using same computer. In the case of MODE-FA and MODE-ACRFA, the required computational time is larger due to larger population size and MNG. Hence, strategy A using Solver for sequential solution of equality constraints seems to be better followed by strategy C using adaptive constraints relaxation with FA for simultaneous solution of optimization problems and equality constraints.

Although two MOO test functions with equality constraints are used in this chapter, these problems are small with a few decision variables and constraints, and are easy to solve. Hence, it is difficult to observe the difference in the performance of FA and ACRFA strategies. Many MOO test functions with equality constraints are required for a comprehensive comparison between FA and ACRFA solution strategies. Use of application problems for testing purpose is not easy as it requires process knowledge and due to the unavailability of a true solution. However, owing to the lack of MOO test functions with equality constraints in the current literature, fermentation processes studied in this chapter are recommended for evaluating constraint-handling approaches in stochastic global optimization techniques. These application problems are challenging, with many equality constraints. Pareto-optimal solutions obtained by MODE-Solver with FA are well distributed and satisfy equality and other constraints. These are available in the Excel file on the web site for this book at http://booksupport.wiley.com.

5.7 Conclusions

In this chapter, feasibility approach (FA) and the adaptive constraint relaxation with feasibility approach (ACRFA) were investigated for the solution of MOO problems with equality constraints, bounds on decision variables and inequality constraints. The performance of these approaches is comparable on two test functions, modified to have equality constraints. Three-stage continuous fermentation and three-stage extractive fermentation processes, which contain many equality constraints arising from mass balances, were optimized using three different strategies: solution of equality constraints using Solver with FA for inequality constraints, FA and ACRFA. Of these, MODE-Solver-FA is the most effective to solve both fermentation processes compared to FA and ACRFA. The feasibility approach requires a suitable value for relaxation, which affects the optimization results obtained, and it performed poorly compared to ACRFA on both fermentation processes. Non-dominated solutions obtained by ACRFA have less average absolute constraint violations than those obtained by FA, and are closer to those obtained by the Solver-FA strategy.

The sequential solution of the optimization problem and equality constraints using Solver along with FA for inequality constraints, is the better strategy for the optimization of the fermentation processes considered here. However, it may not be efficient if the solution of equality constraints (i.e., process model equations) is computationally intensive. In such cases, the simultaneous solution of the optimization problem and equality constraints via the ACRFA strategy may be suitable. Further research is required to improve ACRFA. Interestingly, there are no benchmark test functions for MOO with equality constraints; but, many chemical engineering applications involve equality constraints. Hence, there is a need for benchmark test functions for MOO with equality constraints. For the present, the fermentation processes studied in this chapter are recommended for testing new strategies for solving equality-constrained MOO problems. For this, equations in these problems and the non-dominated solutions obtained are readily available in the Excel file provided on the book's web site.

Acronyms

AACV	average absolute constraint violation.
ACRFA	adaptive constraint relaxation with feasibility approach.
FA	feasibility approach.
GD	generational distance.

HDE	hybrid differential evolution.
MNG	maximum number of generation.
MODE	multi-objective differential evolution.
MOO	multi-objective optimization.
MO-PSO	multi-objective particle swarm optimization.
NSGA-II	non-dominated sorting genetic algorithm-II.
SOO	single objective optimization.
SPEA2	strength Pareto evolutionary algorithm.
TACV	total absolute constraint violations.
TL	tolerance limit (used with MODE-FA solution strategy).

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