APPLICATIONS of MULTIOBJECTIVE OPTIMIZATION

in

CHEMICAL ENGINEERING

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ABSTRACT

Multiobjective optimization involves the simultaneous optimization of more than one objective function. This is quite commonly encountered in Chemical Engineering. A considerable amount of research has been reported in this area over the last twenty years. These are reviewed in the present paper. The general background of this area is presented at the beginning, followed by a description of how the results can be described in terms of Pareto sets. We then present the several methods available for generating these optimal solutions. Applications of optimization in Chemical Engineering wherein multiple objectives are encountered, as well as special adaptations of the basic algorithms required to solve these problems, are then discussed. Some comments are also made on possible directions that future research may take in this area.

Keywords: Multiobjective optimization, Pareto sets, ε-constraint technique, Genetic Algorithm, Non-dominated sorting genetic algorithm.

1. INTRODUCTION

Present day chemical engineering is associated with core competencies in four major areas: reaction engineering, transport phenomena, separations science, and computational and systems science. Several paradigm shifts have taken place in this discipline over the years. These include the introduction of mathematical modeling in its various forms (including process control, systems approach, etc.), the shift from unit operations to transport phenomena, the recent transition towards biosystems, etc. However, one facet of chemical engineers remains unchanged, namely, that they have a responsibility of integrating the chemical engineering core constituencies with economic parameters so as to achieve commercial success. In this context, optimization of chemical processes plays a key role in chemical engineering. Optimization techniques have been applied to problems of industrial importance ever since the late 1940s and several excellent texts (Beveridge and Schechter, 1970; Bryson and Ho, 1969; Edgar and Himmelblau, 1988; Lapidus and Luus, 1967; Ray and Szekely, 1973) describe the various methods with examples. The complexity of the problems studied has increased as faster and more powerful computational hardware and software have become available. We believe that solutions of even more sophisticated optimization problems will become available as complex biosystems are studied and get exploited commercially in the future. In this decade, particularly, several industrial systems have been optimized, which involve multiple objective functions and constraints, using a variety of mathematical techniques and robust computational algorithms. In a few cases, the optimal solutions have been implemented in industry with some success. This short review describes these recent studies, and illustrates them with their adaptations and applications. Some conjectures at a conceptual level are

presented thereafter, and it is hoped that these will mature to fruition as more work gets reported in this interesting area of activity.

Optimization of chemical processes has been a fascinating field of study for several decades. Until about 1980, virtually all problems in chemical engineering were optimized using *single* objective functions. Often, the objective function (also called the cost function) accounted for the economic efficiency only, which is a scalar quantity. The reason for solving such relatively simple optimization problems was possibly, the limitations posed by the technology of computing systems. Most real-world chemical engineering problems require the simultaneous optimization of *several* objectives (multiobjective optimization) which cannot be compared easily with each other (are non-commensurate), and so cannot be combined into a single, meaningful scalar objective function. Examples include reliability, safety, hazard analysis, control performance, environmental quality, etc., apart from the major goal of achieving economic efficiency. Until a few years ago, these several objective functions were combined into a single scalar objective function, using arbitrary weightage factors, so that the problem could become computationally tractable. This 'scalarization' of what is really a vector objective function suffers from several drawbacks. One is that the results are sensitive to the values of the weighting factors used, which are difficult to assign on an *a-priori* basis. What is even more important is the less-recognized fact that there is a risk of losing some optimal solutions (Chankong and Haimes, 1983; Haimes, 1977). This happens if the non-convexity of the objective function (a set is said to be convex if the line joining two points of the set lies within that set) gives rise to a duality gap. [Numerically, a duality gap is the difference between the primal and the dual objective values (Farber, 1986; Goicoechea et al., 1982). Dual is another mathematical program with

the property that its objective is always a bound on the original mathematical program, called the primal. If the primal is feasible, the dual cannot be unbounded, and vice versa; if the dual is feasible, the primal cannot be unbounded. A dual provides a sufficiency test for optimality, for if feasible x and y can be found such that f(x) = F(y), it follows that x is optimal in the primal and y is optimal in the dual]. Therefore, it is necessary that a *vector* form of all the objective functions be used in formulating and solving real-life optimization problems. Such multiobjective optimization problems form the subject of this review.

The concept of multiobjective optimization is attributed to the economist, Pareto (1896). After several decades, this concept was recognized in operations research and has recently become popular in engineering. Extensive literature is now available on multiobjective optimization but we limit ourselves to problems of Chemical Engineering interest only.

We start with a discussion of a simple example of a multiobjective optimization problem to illustrate some elementary concepts. Most techniques of solving such problems comprise of two phases---an objective phase, which is more precise and mathematical, followed by a subjective phase, which is statistical in nature and involves intuition and interaction with human beings (called decision-makers, DMs) who are familiar with the industrial operation being studied. In the first phase, a *set* of several optimal solutions is generated. This is referred to as the Pareto set. For example, a typical two-objective function minimization problem can be represented mathematically as

$$\text{Min } \mathbf{I}(\mathbf{x}) \equiv [\, I_1(\mathbf{x}), I_2(\mathbf{x})] \qquad \text{(a)}$$

subject to (s.t.):

Model equations; (b)

$$g_j(\mathbf{x}) \leq 0, \qquad j = 1, 2, \ldots, J; \qquad (c)$$

$$h_k(\mathbf{x}) = 0, \qquad k = 1, 2, \ldots, K; \qquad (d) \qquad (1)$$

In Eq. 1, **x** represents a p-dimensional set (vector) of p design or *decision* variables. One needs to obtain the optimal values of **x**, which will minimize the two individual objective functions, I_1 and I_2 (which are constituents of the vector, **I**), while satisfying the requirements on g_j and h_k. $g_j(\mathbf{x})$ and $h_k(\mathbf{x})$ represent several inequality and equality constraints which limit the choices of **x**.

It is found that the solution of Eq. 1 often (but *not* always) comprises of *several* sets of optimal values of **x**, and is not necessarily a unique, single point in the p-dimensional **x**-space. These several solutions correspond to different values of I_1 and I_2. Figure 1 shows the optimal solutions of Eq. 1 schematically, for a typical problem. Each point in the I_2 *vs.* I_1 plot in Figure 1 corresponds to an optimal solution, **x** ($\equiv[x_1, x_2, \ldots, x_p]$) of Eq. 1. The curve in Figure 1 is referred to as the Pareto set (Chankong and Haimes, 1983). If we consider two points, A and B, on this Pareto set, we find that on moving from one to the other, one objective function improves (decreases) while the other one worsens (increases). It is, therefore, not possible for us to identify which of these two points is superior to the other. Such points are called as non-inferior or non-dominating points since they are equally good. More formally and generally, non-inferior (or non-dominating) points are those for which, on moving from one point to the other, an improvement in one objective function cannot be obtained without deterioration in the other. Of course, several additional solutions, **x**, also exist which satisfy all the constraints in Eq. 1, but these are not optimal in any manner, and are excluded from Figure 1, since these are inferior to (or are dominated over by) the points shown in this diagram. We illustrate this using point C. If we compare

points A and C, we observe that these two points are non-dominating. However, point C is not a member of the Pareto set because point B is superior to C in terms of *both* the objective functions. The Pareto set narrows down the choices available to a decision-maker, who has to consider only these points for *further evaluation*. The Pareto set is obviously the first step for an optimization problem and is extremely useful.

Point, U, in Figure 1, is referred to as the utopia. This is the point at which the two asymptotes of the Pareto set, meet. The asymptote, $I_i = I_i^* = \text{constant}$, can be obtained by solving the single objective function optimization problem in which we minimize *only* $I_i(\mathbf{x})$. Thus, Eq. 1a is replaced by Min $I_i(\mathbf{x})$, with Eqs. 1b-d unchanged. It is clear that point U is not a solution of Eq. 1 [else it would have dominated over all the points of the Pareto set, and would have been the only (unique) solution to the problem], but represents an 'ideal'. This point is a reference point used quite often for comparing optimal solutions. Pareto sets where one objective function is to be minimized while the other is to be maximized, or where both the objective functions are to be maximized, can be drawn in a manner similar to Fig. 1. In this review, however, we will discuss problems involving the minimization of *all* the objective functions only. This does not lead to any loss of generality since it is known (Deb, 1995) that one can easily replace the maximization of any objective function, say, I_i, by the minimization of a function, F_i. Several possible functions could be used (which do not change the location of the optima), and a simple and popular transformation is $F_i \equiv 1/(1 + I_i)$.

A classic example of a 2-dimensional Pareto set (two-objective function problem) in Chemical Engineering is provided by an isothermal batch reactor in which the following series reaction is taking place:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

(2)

We are interested in maximizing *both* the yield and the selectivity of the desired product, B, simultaneously. These are defined by

$$\text{Yield of B} = \frac{\text{mol of desired product, B, produced}}{\text{mol of reactant fed}}$$

$$\text{Selectivity of B} = \frac{\text{mol of desired product, B, produced}}{\text{mol of all products formed}} \qquad (3)$$

Maximization of the yield is important since it leads to higher amounts of B. Maximization of the selectivity is desired since it leads to a reduction in the downstream separation costs. The yield and selectivity can be computed quite easily as a function of time, t, for any feed and temperature, by integrating the mass balance equations for this system. If we consider the simple problem where t is the only decision variable, and select a feed of pure A, and with temperature selected such that $k_2/k_1 = 0.1$ and $k_1 = 0.1$, we obtain the results shown in Figure 2 (curve PQR, for $0 \leq t \leq 50$). In region PQ, point Q dominates over all the other points and so would be the natural choice for the point of operation. However, the choice of the operating point is not as easy in region QR. In this region, one objective improves and the other worsens as we move from one point to another. Thus, QR is the Pareto set of equally good, optimal points for this problem. The associated values of the decision variable, t, for each of these points is also shown in Figure 2. The choice of the operating point is to be decided based on some *additional* criteria. Point U represents the utopia. The existence of a Pareto set even in such simple problems is not usually recognized or

discussed in Chemical Engineering texts. Some more classical multiobjective optimization problems in Chemical Engineering have been presented by Seinfeld and MacBride, 1970; Nishitani and coworkers, 1979, 1980, 1981; Shieh and Fan, 1980; Umeda et al., 1980 and Grossmann et al., 1982.

The generation of the Pareto set (QR in Figure 2) was quite easy, and was done using qualitative arguments once the yield *vs.* selectivity plot (PQR in Figure 2) was obtained by integrating the mass balance equations. No sophisticated optimization algorithm was required for this simple problem. Several techniques are available to generate the Pareto sets for the more general problems. These are discussed later in this review.

The generation of the Pareto completes the more precise Phase I of the optimization process. In the more subjective Phase II of the study, one has to use additional information that is often intuitive and non-quantifiable in nature, to choose an operating point from among the entire Pareto set, for operation. This point is referred to as the preferred solution. A few methods are available for obtaining this point. One is to ask several decision-makers to rank the points on the Pareto set on a 10-point scale, using their intuition or 'gut' feeling. A weighted-average ranking is then computed and the 'best' point is selected. This second phase of the optimization procedure is not discussed here in too much detail.

It is to be noted that multiobjective optimization is becoming quite popular in Chemical Engineering. In this review, we shall attempt to describe the various techniques and their adaptations, which have been used to obtain the Pareto solutions for several interesting and complex problems of interest to chemical engineers. It is hoped that this review would spur more activity in this area and also help in the recognition of Pareto sets

where these have, indeed, been obtained by experimentation or simulation. Table 1 summarizes the several multiobjective optimization problems studied in Chemical Engineering and classifies them into different areas. Table 2 provides more details on the techniques used for optimization, methods used for the generation of the non-inferior Pareto set and for decision-making, and also gives some important comments on the problem studied.

2. TECHNIQUES OF GENERATING PARETO SETS

Extensive research has been reported on the algorithms used for generating the non-inferior Pareto solutions. These are described in several textbooks (Zeleny, 1974, 1982; Cohon, 1978; Hwang and Masud, 1979; Steuer, 1986; Haimes et al., 1975, 1990; Chankong and Haimes, 1983; Goicoechea et al., 1982) and research and review articles (Geoffrion, 1967a-c; Geoffrion et al., 1972, Zionts and Wallenius, 1976, 1980, Hwang et al., 1980, Clark and Westerberg, 1983, Srinivas and Deb, 1995). We present a short summary of the different techniques used.

2.1 Utility Functions

In this technique, one defines a scalar utility function, u(**I**), of the different objective functions, I_1, I_2,…, I_n:

$$u(\mathbf{I}) = f(I_1, I_2, ..., I_n) \tag{4}$$

The utility function is optimized to obtain the preferred solution. The utility function is an abstract variable indicating goal attainment. For a chemical engineer, the objectives in a typical industrial setting could either be quantifiable quantities, as, for example, minimization of the cost of production while meeting specifications on the products and

effluents, etc., or, a decision maker (DM) could define the utility to include intuitive quantities, e.g., operability and controllability of the plant, reliability of the process, etc. In this interpretation, the possibility of measuring the utility does exist, though formal techniques are not available. Thus, the utility is a way of allowing the decision maker to describe his goals in an abstract way. The drawback of this technique is that the utility function, usually, cannot be determined systematically (Haimes et al., 1975). No Chemical Engineering examples have been solved using this method, to the best of our knowledge.

2.2 Indifference Functions

This method is based on a relative comparison of the objectives. The DM is expected to specify the preference of one objective over the other. Indifference functions/curves (Chankong and Haimes, 1983) are usually plotted to obtain the relative worth of the individual objective functions. The indifference trade-off or the marginal rate of substitution (which is always present for any two points on the indifference curve) is defined as the amount of degradation of one objective the DM is willing to tolerate in exchange for the amount of improvement in the other objective while the preferences for the two points on the indifference curve remain the same. The application of this technique is limited to a maximum of two or three objectives, since a geometrical representation and analysis is required. Some form of reduction of the dimensionality is necessary when there are more than three objective functions, which makes this procedure quite cumbersome. Again, this technique has not been applied to problems in Chemical Engineering.

2.3 Lexicographic Approach

The objective functions are classified (by ‘priority’) by the DM and the preferred solution is defined as that which simultaneously optimizes as many of the objectives as

possible, *hierarchically*. The DM is asked to rank the criteria in terms of decreasing importance (say, I_1, I_2,…, I_n). Only the alternatives that yield the most 'preferred' value for I_1 are used for further evaluation. This solution set is used for the next round to get the most preferred value of I_2. This procedure is repeated until all the criteria are satisfied to yield the best solution. If the best solution is not unique, then additional attributes are used to choose the best solution. This approach generated considerable interest because it mimics the process of human decision-making. But the problem with this approach is that the solution is very sensitive to the ranking of the objectives by the DM and, therefore, one should be careful in applying this technique to objectives having almost equal importance. Different results may be obtained for such cases depending upon the ranking of such objectives by the DM [Haimes et al., 1975; Chankong and Haimes, 1983]. Recently, the lexicographic technique was used by Meadowcraft et al., 1992, for the design of a modular multivariable controller (MMC). Both steady state and dynamic characteristics were considered. The controller thus designed could handle the list of desired operational objectives, re-prioritization of the control objectives and constraints. The controller also provided explicit fault-tolerant control in the presence of instrument failures and allowed manual control of the failed subsystems. The controller finds the solution where as many objectives are satisfied as possible, in order of importance, by using a combination of lexicographic technique and the generalized goal programming approach (discussed in Sec 2.6). Inequality constraints are classified into *hard* and *soft* constraints depending on their relative importance to the other objectives and are incorporated into the design procedure.

2.4 Parametric Approach

This is the simplest of all the techniques. The objective functions, I_i, are combined into a single overall scalar objective, I:

$$I = \sum_{i=1}^{n} w_i I_i(\mathbf{x})$$

$$0 \leq w_i \leq 1 \qquad (5)$$

$$\sum_{i=1}^{n} w_i = 1$$

where $\mathbf{x} \in \mathbf{X}$, $\mathbf{X}$ being the feasible optimum region. A non-inferior point is generated by changing the relative weights, w_i. The solutions may be viewed as points in the optimum search-space that offer the least conflict among the objectives. Least conflict is possible when the weights used are equal for all the objectives, which is not a practical, satisfying solution for a real system. The relative weights need to be assigned to each of the objective functions based on the individual optimum solution. The major drawback of this technique is that it cannot generate the entire non-inferior set when "duality-gaps" exist, which means that the problem is non-convex (Haimes et al., 1975; Chankong and Haimes, 1983; Srinivas and Deb, 1995). It is well known that verifying the convexity requirement for large-scale systems is quite difficult. Also, for such systems, *a-priori* knowledge of the weights is practically not possible. Though this method gives a solution to the overall objective, the insight into the conflicts among the objectives is lost in the process. Some of the classical examples in Chemical Engineering have used the parametric approach in solving the multiobjective problem. Seinfeld and MacBride, 1970 have used a modification (Geoffrion, 1967c) of this method to minimize the parametric sensitivities in a refinery. A simplified refinery model was formulated and the objectives considered were (i) maximization of the

total yearly profit and (ii) minimization of the sensitivity of the profit to variations in refinery conditions. Ten constraints (both equality and inequality) were imposed and twelve decision variables were considered in this study. Fan et al., 1984, have used this approach in the optimization of batch polymerizations involving chain propagation with monomer termination. Trade-offs among the monomer conversion and the mean and the standard deviation of the molecular weight distribution (MWD) of the polymer, have been explained using a triangular graph. Though the method is fairly simple to use, the accuracy of the solution is not guaranteed.

2.5 The ε-Constraint Approach

This approach is one of the most popular methods that have been applied for solving multiobjective optimization problems. This technique was proposed by Haimes et al., 1971 and is described in detail by Haimes et al., 1975 and Chankong and Haimes, 1983. This technique does not require the existence of supporting hyper-planes and overcomes duality-gaps in non-convex sets. These advantages have made this approach very useful and popular.

In this technique, we optimize a *single* objective function (chosen from among the original ones) while treating all the remaining objectives as inequality constraints. A multiobjective optimization problem defined similar to the two-objective function problem defined in Eq. 1 is, thus, reformulated in this technique as

$$\text{Min} \quad I_1(\mathbf{x})$$

s.t.:

$$I_i(x) \le \varepsilon_i \qquad i = 2, 3, \ldots, n$$

$$g_j(\mathbf{x}) \le 0 \qquad j = 1, 2, \ldots, J$$

$$h_k(\mathbf{x}) = 0 \qquad k = 1, 2, \ldots, K \qquad (6)$$

It is to be mentioned that *any one* of the n objective functions, $I_1, I_2, \ldots, I_n$, can be selected as the single objective function to be minimized (and is referred to as I_1) [we shall assume that all the objective functions are to be minimized, since maximization problems can easily be transformed into minimization problems, as discussed earlier].

By varying the constraint-levels, ε_i , one can generate the entire Pareto optimal hyper-surface in the n-dimensional **I**-space. The minimum values of the individual ε_i have to be obtained by solving simpler, 1-objective function optimization problems (Chankong and Haimes, 1983). Any appropriate technique can be used to solve the optimization problem in Eq. 6. It is clear that this simpler optimization problem (Eq. 6) has to be solved several times to generate the Pareto set, and so this method is quite compute-intensive.

Three different adaptations of this technique are available: the equality constraint approach, the inequality constraint approach and the hybrid (weighting-constraint) approach. The equality constraint has the added advantage that *analytical* solutions for small-size problems can be obtained. Wajge and Gupta, 1994a, used this form to optimize a non-vaporizing nylon 6 batch reactor. They minimized the (i) reaction time, t_f, and (ii) concentration, $[C_2]_f$, of the undesired side product, the cyclic dimer, in the product, while requiring the monomer conversion and the number average chain length in the product to lie at design or desired values ($x_{m,d}$ and $\mu_{n,d}$, respectively). The temperature history, T(t), was used as the decision variable. Pontryagin's minimum principle was used with the first-order control vector iteration method (Ray and Szekely, 1973) to solve the problem with the ε-equality constraint incorporated. These workers reported some numerical oscillations in the Pareto sets. They also encountered convergence problems when using larger values

of ε. Sareen and Gupta, 1995, used the same objective functions and end-point constraints (on the product) to optimize an *industrial* semi-batch nylon 6 reactor. In this reactor, monomer and water vaporize and build up the pressure in the vapor space above the liquid reaction mass, at a rate depending on the release of the vapor mixture through a control valve. They used the jacket-fluid temperature, T_J (a scalar *value*), as well as the pressure history, p(t) (a continuous *function* of time, t), in the reactor as the decision variables. The pressure history was parametrized (shape fixed) and was represented in terms of five parameters (*constants*, rather than a *function).* Sequential quadratic programming (SQP), developed by Gill et al., 1981 (which has a first-order convergence), was used for solving the single objective function problem obtained with the ε-equality constraint method. Some amount of scatter was obtained in the Pareto set. A 'smoothening procedure' was used to get sub-optimal but smoother Pareto sets. Substantial improvements in the operation of the industrial reactor were indicated when operating the reactor at *any* of the points on the Pareto set.

The inequality form in Eq. 6 is very useful when the DM wishes to solve the problem interactively. The Kuhn-Tucker (positive) multipliers associated with the optimization problem reflect the sensitivity of the primary objective, I_1, to the active constrained objectives, I_i, and so give an indication of the trade-offs among the objectives. The values of the Kuhn-Tucker multipliers indicate the price that one needs to pay in terms of one objective, if one wishes to improve another, while still remaining on the non-inferior set. The drawback of this technique is that the test of non-inferiority needs to be performed. This leads to an increase in the computational time. This method also locates some of the points that are *inferior* (Chankong and Haimes, 1983; Clark and Westerberg, 1983). This

method has been used extensively (Sophos et al., 1980; Tsoukas et al., 1982; Fan et al., 1984; Farber, 1986; Palazoglu and Arkun, 1986; Videla et al., 1990; Luyben and Floudas, 1994 a, b) in Chemical Engineering.

Sophos et al., 1980, optimized a petrochemical industry using multiple objectives. These were to optimize (i) the energy utilization (which included maximization of the change in the thermodynamic availability and minimization of lost work) and (ii) carbon utilization efficiency (which is equivalent to minimization of the feed stock consumption). Compromise 'bounding structures' (optimal solutions of each objective) were generated for the system studied. The two objectives given above were considered first and a Pareto set was obtained between the feed consumption and the lost work. Pareto surfaces were also generated for a three objective function problem using linear programming. Two preferred solutions were identified from the Pareto surface. In one case, the method used was goal programming (discussed in Section 2.6) while in another, commensuration of the objective functions for a *specific case* was used before solving a single objective function optimization problem.

Tsoukas et al., 1982, were the first to introduce the concept of multiobjective optimization in polymerization reactors, where the presence of conflicting objectives is common. Pareto optimal solutions were determined for the dual objectives of (i) narrowing the copolymer composition and (ii) narrowing the molecular weight distribution for styrene-acrylonitrile (SAN) copolymerization in a semi-batch reactor. Temperature, initiator concentration and monomer addition histories (functions of time) were used as the decision variables. Farber, 1986, extended this work to continuous copolymerization reactors. They considered both methyl methacrylate-vinyl acetate (MMA-VA) as well as

SAN systems. Pareto sets were obtained [composition *vs.* molecular weight; conversion *vs.* molecular weight] for the MMA-VA system using the temperature history of the reactor as the decision variable. In the SAN system, a Pareto optimal set was obtained for conversion *vs.* molecular weight by using both temperature history and residence time as decision variables. Fan et al., 1984, also used this technique for chain polymerizations in a batch reactor (the same as discussed in the previous study) and compared the results with those obtained using the parametric approach.

Palazoglu and Arkun (1986) studied the problems of operability associated with improper design, modeling and control system design in the presence of uncertainties. They proposed a process design methodology to find optimal operating regions for chemical units. This approach guides the designer towards process designs with improved dynamic operability and economics. Characterization of dynamic operability was done using an index for robustness. The ellipsoid algorithm (Ecker and Kupferschmidt, 1983) was used for solving the optimization problem interactively. The optimization problem consists of non-linear problems with an infinite number of constraints that are frequency dependent, and are handled using a discretization procedure developed by these workers. A symbolic logic language, MACSYMA, was used to get the design variables transferred from the non-linear plant equations to the transfer function, thereby avoiding successive linearizations. A system of three isothermal CSTRs was used as an example.

A modified ε-constraint approach has been used for the optimization of an anaerobic digester treating the leachate from a controlled solid urban waste landfill. Videla et al., 1990, considered the (i) maximization of the net production of energy from biogas, (ii) maximization of the percentage removal of chemical oxygen demand (COD), and (iii)

minimization of the capital outlay, as the three objective functions. The constraints imposed were

(i) the percentage COD removal must be at least 50%;

(ii) the digester must treat a specified flow rate of leachate per day; and

(iii) all the individual objective functions must be positive.

The decision variables were the residence time, the temperature of operation and the diameter to height ratio. The weighted sum of the deviations from the respective optima of the *individual* objective functions was minimized. Pareto optimal solutions were generated for the net biogas production *vs.* the percent COD removal, for different volumes of the digester. An interactive, iterative optimization procedure, based on the solution of the non linear programming (NLP) problems was used to obtain the preferred solution for the two cases. The first of these involved the minimization of the cost while the other involved the maximization of the net energy production with at least 75% of COD removal.

Luyben and Floudas (1994 a, b) analysed the interaction between process design and control using a multiobjective framework for two example systems, a binary distillation system and a reactor-separator-recycle system. They proposed a systematic approach to determine both the steady-state economic and open-loop controllability objectives within the mathematical programming framework of process synthesis. The possible design alternatives were translated to a multiobjective mixed-integer non-linear optimization problem. A non-inferior solution set was determined by applying the ε-constraint technique within the framework of the generalized Benders' decomposition (Geoffrion, 1972; Paules and Floudas, 1989). A method based on the cutting plane algorithm (Geoffrion et al., 1972) was used to determine a best-compromise solution by the knowledge of trade-off weights

among the economic and control objectives. As explained earlier, this information is obtained by the partial derivatives from the non-inferior set. This procedure was applied for binary distillation synthesis involving multiple objectives, control configuration selection and possible heat integration. They also applied this procedure for the multiobjective optimization of a recycle system consisting of a reactor followed by a distillation column, where the distillate is recycled to the reactor. A non-linear model incorporating all possible design variables was used for optimization. It was found how specific changes in design affect both the economic and control objectives. The conflict between the process and disturbance gains was very well exhibited by the non-inferior solutions.

The third type of the ε-constraint approach is the hybrid form that combines the principles of the parametric approach with the ε-constraint technique. The hybrid form can be represented as

$$\text{Max/Min} \quad \mathbf{w}^T\mathbf{I}(\mathbf{x})$$

subject to:

$$0 \le w_i \le 1$$

$$\sum_{i=1}^{n} w_i = 1$$

$$I_i(\mathbf{x}) \le \varepsilon_i$$

$$g_j(\mathbf{x}) \le 0 \qquad j = 1,2,\ldots, J$$

$$h_k(\mathbf{x}) = 0 \qquad k = 1,2,\ldots, K \qquad (7)$$

The hybrid form does not require any non-inferiority tests and is, therefore, more efficient when the user is interested in generating *only* the Pareto optimal solutions numerically. Interactive decision making is not possible with this method.

Though the ε-constraint technique can also be used to solve problems which are non-convex, the difficulty with this method is that an *a-priori* knowledge of the appropriate range of values of ε_i , is required.

2.6 Goal Programming (Charnes and Cooper, 1961)

A preferred solution is obtained by minimizing a weighted average deviation of the objective functions from the goals set by the DM. This is represented mathematically as

$$\text{Min } I = \left[\sum_{i=1}^{n} \left(I_i(\mathbf{x}) - y_i \right)^r \right]^{1/r}, \quad 1 \le r < \infty \qquad (8)$$

where $\mathbf{x} \in \mathbf{X}$ (the feasible region), and y_i is the goal or the demand-level of the ith objective. Usually, r takes the value of 2 with y_i as the individual optimum of the ith objective. This represents the root mean square deviation from the goals. The arbitrary selection of the demand-level vector leads to a non-Pareto optimal solution. Equal weights for all the deviations of the objectives are normally assumed, as was assumed in Eq. 8. If weights are introduced, then the problem of a duality gap arises when the problem is non-convex. Also, the DM has to be aware of the individual optimum of each objective prior to the selection of the values of the demand levels.

A variation of this technique is the min-max formulation to solve multiobjective optimization problems. Nishida et al., 1974, formulated and solved the synthesis problem as a min-max formulation within the framework of optimal control. The objective of this method was to minimize the relative deviations from the individual optimum of the single objective functions, when $r = \infty$. The method tries to minimize the objective conflict. The best compromise solution is obtained when objectives with equal importance are optimized.

This method also suffers from the drawback of duality gaps and sometimes it locates solutions which are inferior.

The technique of goal programming has been applied in Chemical Engineering by Kraslawski et al., 1991, Kraslawski and Pustelnik, 1991 and Smilgielski et al., 1992. Kraslawski et al., 1991, have used this technique for optimizing the operating conditions for self-sucking impellers in a bioreactor. The objectives were to (i) minimize the mixing power requirement and (ii) to maximize the mass transfer coefficient. The decision variables were the rate of rotation of the impeller, and the diameter to height ratio of the tank. The problem was transformed to a min-max formulation and the fuzzy weights determined based on the 'linguistic' variables (qualitative information such as small, large, very small, very large, etc.) used in the problem.

The min-max problem-formulation was also used by Kraslawski and Pustelnik in determining the optimum values of the number of elements and the flow velocity for a kenics static mixer. The two objective functions used were: (i) minimization of the pressure drop and (ii) the maximization of the degree of mixing. The optimal solution was obtained by a sequentially-built compromise function method, which prioritizes the objective functions (a form of lexicographic approach) *a-priori*. Both the methods used experimental data and the simplex method to arrive at the optimal solution. The min-max formulation uses the weights decided by the DM whereas the latter method considers the solution to be feasible if the degree of mixing (first priority) attains 99% of the maximum degree of mixing. A complete analysis needs to be made by changing the weights and the priority levels to give an understanding of the non-inferior solutions. The reader does not get any insight about the nature and extent of the conflict between the two objectives in this case.

A multiobjective optimization study (using experiments) was carried out by Smigielski et al., 1992, on the electrochemical reduction of maleic acid to succinic acid. The objectives were to (i) maximize the degree of inversion and (ii) minimize the wastes produced in the process. The decision variables used were the concentrations of maleic acid and sulphuric acid, current intensity, temperature, and the electric charge. The optimum operating point was achieved by formulating a goal-programming problem, where the demand-level vector consists of values of the utopia of the individual objectives. Fuzzy set theory was applied to get the weights in the objective function. The method is termed as the utopia-point method. The simplex method was used to arrive at the best compromise solution. Based on investigations on a pilot plant, a design was suggested for the continuous production of succinic acid. This work did not use any mathematical model for the optimization. It used, instead, data obtained from experiments. The data did not cover the entire feasible region.

2.7 Genetic Algorithm (GA)

GA is a search technique developed by Holland (1975) that mimics the process of natural selection and natural genetics. In this algorithm, we code a set of values of the decision variables (a solution, **x**) in terms of a 'string (or chromosome)' of binary numbers, generated using random numbers. A 'population (gene pool)' of such binary strings is first generated. Each chromosome is then mapped into a set of *real* values of the decision variables, using the upper and lower bounds of each of these. This ensures that the decision variables lie within their bounds. Then, a model of the process is used to provide values of the objective function for each chromosome. The value of the objective function of any chromosome reflects its 'fitness'. The Darwinian principle of 'survival of the fittest' is used to generate a new and improved gene pool (new generation). This is done by preparing a

‘mating pool’, comprising of copies of chromosomes, the number of copies of any chromosome being proportional to its fitness (Darwin's principle). Pairs of chromosomes are then selected randomly, and pairs of daughter chromosomes generated using operations similar to those in genetic reproduction. The gene pool evolves, with the fitness improving over the generations.

GA is noted for its robustness. This algorithm is superior to traditional optimization algorithms in many aspects, and has become quite popular in recent years. It is better than calculus-based methods (both direct and indirect methods) that generally seek out the local optimum, and which may miss the global optimum. Most of the older techniques require values of the derivatives of the objective functions, and quite often, numerical approximations of the derivatives are used for optimization. In most real-life problems, the existence of derivatives is questionable and often, the functions are discontinuous, multi-modal and noisy. In such cases, calculus-based methods fail. Enumerative schemes, which are based on the point-by-point comparison of the values of the objective function in a discretized infinite (or even a finite) search space, are inefficient for large problems since the search space is often, too large. Random search techniques, too, suffer from a similar disadvantage since they work like enumerative techniques in the long run. GA is superior to these techniques since it is conceptually different from these traditional algorithms in several respects. It uses a population of several points *simultaneously*, as well as works with probabilistic (instead of deterministic) operators. In addition, GA uses information on the objective function and not its derivatives, nor does it require any other auxiliary knowledge.

Three common operators are used in GA [called simple GA (SGA), to distinguish it from its various adaptations] to obtain an improved (next) generation of chromosomes. These are referred to as reproduction, cross-over and mutation. Reproduction, as described above, is the generation of the mating pool, where the chromosomes are copied probabilistically, based on their fitness values. Then, a pair of daughter chromosomes are produced by selecting a cross-over site (chosen randomly) and exchanging the two parts of the pair of parent chromosomes (selected randomly from the mating pool), as illustrated below for two chromosomes carrying information about three decision variables, each represented by four binary digits:

$$\begin{array}{lcl} 1001\ 1 \vdots 100\ 0111 & & 1001\ 1 \vdots 101\ 1100 \\ 0011\ 0 \vdots 101\ 1100 & \Rightarrow & 0011\ 0 \vdots 100\ 0111 \\ \text{parent chromosomes} & & \text{daughter chromosomes} \end{array} \qquad (9)$$

In Eq. 9, the crossover site for *this* pair of parent chromosomes is taken just after the fifth binary digit. It is hoped that the daughter strings are superior. If they are worse than the parent chromosomes, they will slowly die a natural death over the next few generations (the Darwinian principle at work).

The mutation operator is required for the following reason. In Eq. 9, let us assume that *all* the chromosomes in the gene pool have a 0 at the second position. There is a finite probability of this happening, since the generation of the binary numbers is done probabilistically. It is obvious that cross-over will never be able to generate chromosomes with a 1 at this position, and if it so happens that the optimum is, indeed, located at a point described by such a chromosome, GA will be unable to reach this solution. The mutation operator looks at *each* binary digit in *every* daughter chromosome in the gene pool, and

transforms a 0 into a 1 (or vice versa) with a small probability. In effect, it moves the chromosome *locally* in the **x**-space, to create a better chromosome. The entire process is repeated till some termination criterion is met (the specified maximum number of generations is attained, or the improvements in the values of the objective functions become lower than a specified tolerance). A more elaborate description of SGA is available in Holland, 1975, Goldberg, 1989, and Deb, 1995.

We now turn our attention to extensions of SGA to solve problems involving multiobjective optimization. Since GA uses a population of points, it seems very natural to use GA for such problems to capture a number of solutions *simultaneously*. Schaffer (1984) was the first to apply an adapted vector evaluated genetic algorithm (VEGA) to solve multiobjective optimization problems. Though it was simple to implement, the method has a bias towards some Pareto-optimal solutions (Goldberg, 1989; Srinivas and Deb, 1995). In order to overcome this problem of bias with some of the optimal solutions, Goldberg proposed a non-dominated sorting procedure. The idea was implemented in different ways by Fonseca and Fleming (1993), Horn et al. (1994) and Srinivas and Deb (1995). The algorithm implemented by Srinivas and Deb (1995) is called the non-dominated sorting genetic algorithm (NSGA). It is to be noted that NSGA overcomes the pitfalls of the previous two techniques (Fonseca and Fleming, 1993, Horn et al. 1994). Fonseca and Fleming (1998 a, b) have recently extended their algorithm, applying the principles of niche and sharing. The concept of non-dominated sorting is first discussed and then we turn our attention to the applications of this technique in Chemical Engineering. It is interesting to note that most of the recent applications in Chemical Engineering have used NSGA (*adapted* as required by the problem).

NSGA uses a ranking selection method to emphasize the good points and a niche method to create diversity in the population without losing a stable sub-population of good points. Principally, NSGA differs from SGA *only* in the way of selection. A check for non-dominance is first carried out among *all* the chromosomes in the gene pool before reproduction is performed. All the non-dominated chromosomes from the entire population are first identified and assigned a front number (Front No. = 1). These non-dominated chromosomes are then assigned a *dummy* fitness value (which is usually the number of chromosomes, N_p, but could be any other arbitrarily selected, large value instead). The dummy fitness value of any chromosome in this front is then modified according to a sharing procedure (Goldberg and Richardson, 1987; Deb, 1989; Deb and Goldberg, 1991) by dividing it by the niche count of the chromosome. The niche count of a chromosome represents the number of neighbors around it, with distant neighbors contributing less than those nearby. The niche count, thus, gives an idea of how crowded the chromosomes are in the **x**-space . This is obtained, say, for the ith chromosome, by computing its distance, d_{ij}, from another, say, jth chromosome in the **x**-space, and using a sharing function, Sh, as given below

$$\mathrm{Sh}(d_{ij}) = 1 - \left(\frac{d_{ij}}{\sigma_{\mathrm{share}}} \right)^{\alpha}, \text{ if } d_{ij} < \sigma_{\mathrm{share}}; \quad 0, \text{ otherwise} \qquad (10)$$

In Eq. 10, σ_{share}, a computational parameter, is the maximum distance allowed between two chromosomes to qualify as neighbors. Obviously, if d_{ij} is larger than σ_{share}, its contribution to Sh is zero (the jth chromosome is then not considered to be a neighbor of the ith), while if $d_{ij} = 0$, its contribution to Sh is 1. For intermediate values of the distance between the two chromosomes, Sh lies between 0 and 1. Thus, by summing up $\mathrm{Sh}(d_{ij})$ for *all values of j* in

any front comprising of non-dominated chromosomes, one can get an idea of how crowded the ith chromosome really is. This summation is referred to as the niche count of chromosome i. The shared fitness value of chromosome, i, is the ratio of the common dummy fitness value assigned initially to each member of the front, and its niche count. Use of the shared fitness value for reproduction, thus, helps spread out the chromosomes in the front since crowded chromosomes are assigned lower fitness values. This procedure is repeated for all the members of the first front. Once this is done, these chromosomes are temporarily removed from consideration, and all the *remaining* ones are tested for non-dominance. The non-dominated chromosomes in *this* round are classified into the next front (Front No. = 2). These are all assigned a dummy fitness value that is a bit lower than the *lowest* shared fitness value of the previous front. Sharing is performed thereafter. This procedure is continued till all the chromosomes in the gene pool are assigned shared fitness values. The usual operations of reproduction, cross-over and mutation are now performed. It is clear that the non-dominated members of the first front that have fewer neighbors, will get the highest representation in the mating pool. Members of later fronts, which are dominated, will get lower representations (they are still assigned some low fitness values, rather than 'killed', in order to maintain the diversity of the gene pool). Sharing forces the chromosomes to be spread out in the **x**-space. The population is found to converge very rapidly to the Pareto set. It is to be noted that any number of objectives (both minimization and maximization problems) can be solved using this procedure. A flowchart describing this technique is presented in Figure 3 (Mitra et al., 1998; Garg and Gupta, 1999). Additional details about the algorithm, its efficiency over other techniques and some

comments on the choice of the computational parameters to be used in NSGA, are described in Srinivas and Deb, 1995 and Deb, 1989.

NSGA has been used to solve a variety of multiobjective optimization problems in Chemical Engineering in recent years, as for example, in the areas of polymer reaction engineering, catalytic reactors, membrane modules, cyclone separators and venturi scrubbers. Various adaptations of the basic NSGA were made in order to be able to obtain meaningful solutions, and these are described below along with the example problems studied. It is hoped that such a discussion would enable a reader to be able to devise his own adaptations for the problem of interest.

The first application of NSGA in Chemical Engineering was for an industrial nylon 6 semi-batch reactor by Mitra et al. (1998). The industrial reactor model was validated (Wajge et al., 1994b) before it was used for multiobjective optimization. The two objective functions used were to minimize (i) the total reaction time, t_f, and (ii) the concentration, $[C_2]_f$, of the cyclic dimer (an undesirable by-product) in the product. Equality constraints were imposed on the monomer conversion, $x_{m,f}$, in the product stream, as well as on the number average chain length, $\mu_{n,f}$, of the product, so that design values, $x_{m,d}$ and $\mu_{n,d}$, are attained for these. The first constraint was taken care of by adding it in the form of a penalty function (Deb, 1995) to both the objective functions. The objective functions were, thus, modified to

$$\text{Min } I_1 = t_f + w_1[1 - (x_{m,f}/ x_{m,d})]^2 \qquad \text{(a)}$$

$$\text{Min } I_2 = [C_2]_f + w_1[1 - (x_{m,f}/ x_{m,d})]^2 \qquad \text{(b)} \qquad (11)$$

The second equality constraint, $\mu_{n,f} = \mu_{n,d}$, was used as a stopping condition, i.e., integration of the model equations, a set of ordinary differential equations (ODEs), was stopped when

this constraint was met. The decision variables used in this study were (i) the rate of release, $V_T(t)$, of the vapor from the semi-batch reactor (a function of time, t) which influenced the pressure in the reactor, and (ii) the jacket fluid temperature, T_J (a scalar). NSGA had to be adapted to apply to decision variables that were continuous functions of time. This was achieved by discretizing the continuous function into several, equi-spaced (in time) scalar values, $V_{T,i}$; i = 1, 2, …, Q, and constraining the value, $V_{T,i}$, to lie within a small range of the previous value, $V_{T,i-1}$. This ensured that the final continuous function, $V_T(t)$ [obtained by curve-fitting the digitized values] was implementable. Pareto-optimal solutions were obtained for a specified value of the feed water concentration (see Figure 4). These results were compared with the solutions obtained earlier by Sareen and Gupta, 1995, who parameterized the pressure history, and so introduced some artificial constraints into the problem (since the shape of the pressure history was assumed to be fixed). Mitra et al. found that the solutions obtained by NSGA were superior. Interestingly, considerable improvement in the operation of the industrial reactor was indicated by this study, and we understand that these results were implemented on the industrial reactor.

Gupta and Gupta (1999) extended this work on the industrial nylon-6 reactor system to consider the multiobjective optimization of the reactor-cum-control valve assembly. They considered the fractional-opening of the control valve as one of the decision variables (again, a function of time), instead of the rate of release of vapor from the reactor. The second decision variable was the temperature of the jacket fluid, a scalar *value*. The Pareto optimal solutions obtained for this *system* were found to be worse when compared to the solutions obtained by Mitra et al., who had studied the reactor *alone* (see Figure 4). This was because the operation of the control valve, which released the vapors, excluded certain

sets of values of $V_T(t)$, which were permitted in the study of Mitra et al. It is clear that for industrial systems, the optimization of the entire *system* is more valuable than that of its major parts (Aatmeeyata and Gupta, 1998).

Garg and Gupta, 1999, applied NSGA to the multiobjective optimization of free radical bulk polymerization reactors, wherein diffusional effects (the Trommsdorff, cage and glass effects) are manifested. The two objective functions used were the minimization of (i) the total reaction time, t_f, and (ii) the polydispersity index, Q_f, of the product. The manufacture of polymethyl methacrylate in a batch reactor was chosen as the example system. Equality constraints were used on the value of the number average chain length, $\mu_{n,f}$, and the monomer conversion, $x_{m,f}$, in the final product, similar to that for the nylon 6 reactor. Optimal temperature histories, T(t), were generated for a given initiator concentration in the feed. Interestingly, a unique optimal solution, instead of a Pareto set of several optimal solutions, was obtained. This was so for *all* the cases studied. This inference was of considerable importance since a controversy had existed on this point for several years, based on earlier optimization studies that used a scalar objective function comprising of a weighted sum of the two objectives.

Rajesh et al. (1999) carried out the multiobjective optimization of a side-fired steam reformer using NSGA. This is a very important industrial process and there is an inherent trade-off between the objectives. Two objective functions were considered: (i) minimization of the methane feed rate (input to the reformer), $F_{CH4,in}$, for a specified rate of production of hydrogen, $F_{H2,unit}$, from the industrial unit, and (ii) maximization of the rate of production of export steam (which was equivalent to maximization of the flow rate, $F_{CO,out}$, of CO in the syngas). The optimization problem was solved using a pre-validated

model. An equality constraint was used on the rate of production of hydrogen (equated to a desired value), and an inequality constraint was imposed on the maximum wall temperature of the reformer tubes. The decision variables used were: the temperature of the gas mixture at the reformer inlet, pressure at the inlet of the reformer, steam to carbon (in the form of CH_4) ratio in the feed, hydrogen (recycled H_2) to carbon (as CH_4) ratio in the feed, the total molar flow rate of the feed, and the temperature of the furnace gas. Pareto optimal solutions for specified rates of production of hydrogen were obtained (see Figure 5). Comparison of the current operating conditions of the *industrial* reformer studied (point Q in Figure 5, for $F_{H2,unit}$ = 3450 kg/hr) with an arbitrary point, P, on the Pareto set (for the same $F_{H2,unit}$) indicated scope for considerable improvement. In this problem, it was found that *feasible* values of one of the decision variables, the steam to carbon ratio in the feed, were within the bounds specified *a-priori*, and were, in fact, influenced by the values selected for the *other* decision variables. The code for NSGA had, therefore, to be adapted for this problem also. Values of all the decision variables except the steam to carbon ratio were first generated for *every* chromosome, following the normal procedure of mapping with the *a-priori* bounds. The bounds for the steam to carbon ratio were then generated for each chromosome. The substring (of binary digits generated randomly) corresponding to this last decision variable was then mapped into a real number, using these chromosome-specific bounds for each chromosome. Similar procedures can be used whenever the bounds on decision variables are chromosome-specific, and need to be adapted continuously during the computation.

Polyethylene terephthalate (PET) is another commercially important polymer, mostly used in the manufacture of synthetic fibers. Bhaskar et al. (2000a) formulated a

multiobjective optimization problem on the industrial, third stage wiped film reactor used to produce this polymer. The objective functions used in this problem were to minimize the concentrations of two undesirable side products, namely, that of the (i) acid end groups, and (ii) the vinyl end groups, in the output stream. An equality constraint was imposed on the degree of polymerization, DP_{out}, of the product, so as to produce PET having a desired value, DP_d (i.e., $DP_{out} = DP_d$). The acid end group concentration in the product was further restricted to lie below a certain value (an inequality constraint), while the concentration of diethylene glycol end group in the product was restricted to lie in a specified *range* (two inequality constraints). This was consistent with current industrial requirements. The three inequality constraints were taken care of by 'penalty-killing' of the chromosomes that violated these constraints, by adding on a heavy penalty value (10^4) to both the objective functions [similar to those in Eq. 11] when these constraints were violated. The solution of the problem was found to be a unique point, and no Pareto set of optimal solutions was obtained. It must be emphasized that it is almost impossible to predict on an *a-priori* basis whether a Pareto set would be obtained or not in any *complex* multiobjective optimization problem. In fact, our experiences with the *simulation* of this reactor (Bhaskar et al., 2000b) had suggested opposing effects and trends, and we were almost sure that a Pareto set would be obtained! The unique optimal solution was found to be superior to the current operating conditions in the industrial reactor studied. Solutions were generated for a few other choices of the objective functions, as for example, the minimization of the residence time and of the acid end group concentration in the product (which minimizes the concentration of the vinyl end group simultaneously), but Paretos were still not obtained.

The technique of *instantaneously* killing the chromosomes violating the inequality constraints, referred to as penalty killing, could lead to some amount of numerical scatter in the final results. Such scatter is less likely to be present in solutions obtained using the *slow* killing of such chromosomes using the more accepted penalty function method (Eq. 11). This is particularly true for complex problems where some amount of multiplicity and/or insensitivity (of optimal solutions) is present. This was encountered in the PET reactor optimization problem, and the unique solutions obtained for different values of DP_d showed some scatter. The optimal results obtained in such problems can be smoothened out (Bhaskar et al., 2000a; Sareen and Gupta, 1995) for use in industry by solving an optimization problem having a smaller degree of freedom (e.g., one with fewer decision variables). Indeed, Goldberg (1989) has mentioned that GA (and so its various adaptations) could have premature convergence when used on complex problems, but that all the results still lie in the optimal 'region'.

Ravi et al. (2000a) performed multiobjective optimization of a train of identical cyclone separators operating in parallel, to process a specified flow rate of dust-laden gases. They considered two objective functions: (i) maximization of the overall collection efficiency, η_o, and (ii) minimization of the pressure drop, Δp (related to the operating cost). The decision variables used for this problem are the number of cyclones, the diameter of the cyclones, and seven geometric ratios (shape) of the cyclones. The bounds on two of the geometric ratios were adapted (depending on the values selected for some of the other decision variables, chromosome-specific bounds) to ensure that the cyclone shape was physically meaningful. The technique used was similar to what was used in the optimization of the steam reformer. An upper limit was imposed on the inlet velocity of

gases (an inequality constraint). This constraint was implemented using penalty killing, as was done for the PET wiped film reactor optimization problem. Δp *vs.* η_o Pareto sets were obtained (see Figure 6). It was found that the optimal values of the decision variables could not, *at first sight*, be explained physically. This problem is quite common in multiobjective optimization problems associated with a considerable amount of 'freedom'. One then needs to solve *several simpler* multiobjective optimization problems, each with only one, or, at most two decision variables, to find out which of the several decision variables in the original problem are the most sensitive and important in deciding the Pareto set. Such a study leads to considerable physical insight and, at times, even helps in developing appropriate bounds of the decision variables, as well as in selecting appropriate constraints to be used in solving the multiobjective optimization problem, which may not be known too precisely at the beginning. Such detailed studies also help in explaining the scatter that may be present in the final results--both in the Pareto set obtained as well as in the plots of the individual decision variables over the range of objective functions covered by the Pareto set. A similar study is being carried out (Ravi et al., 2000b) on the multiobjective optimization of venturi scrubbers. Pareto optimal solutions are being obtained in the preliminary studies completed till now.

Multiobjective optimization of hollow fiber membrane modules was carried out by Chan et al. (2000), using the dialysis of beer to produce low-alcohol beer, as an example. The two objective functions considered were (i) the maximization of the removal of alcohol from the beer, and (ii) the minimization of the removal of 'taste chemicals (called extract)' by the module. Inequality constraints were imposed on the pressure drops on both the shell and the tube sides, as well as on the inner diameter of the shell. The decision variables

considered were the flow rate of water on the shell side, the length of the fiber, the fractional free area in the shell (related to the tube pitch), the internal radius of the individual hollow fibers and the thickness of the hollow fiber membranes. Again, this problem is associated with an immense amount of freedom, and several simpler one- and two- decision variable problems have been studied to develop physical insight. It was found that the internal radius of the membrane was the most important decision variable influencing the Pareto set.

Another application of considerable industrial importance is the optimization of the continuous casting of polymethyl methacrylate (PMMA) films. In this process, a prepolymer is first produced in an isothermal plug flow tubular reactor (PFTR). The product from this reactor flows as a thin film through a furnace. The temperature, $T_w(z)$, of the upper and lower surfaces of the polymer film varies with the axial location, z, in the furnace. The two objective functions (Zhou et al., 2000) are (i) the maximization of the cross section-average value of the monomer conversion at the end of the furnace, $x_{m,av,f}$, and (ii) the minimization of the length, z_f, of the furnace. The end-point constraint used was that the section-average value of the number average chain length in the product, $\mu_{n,av,f}$, should be equal to a desired value, $\mu_{n,d}$. In addition, a 'local' constraint is to be satisfied in this problem. This takes the form that the temperature at *any* point in the film must be below an upper safe value, to prevent degradation (discoloration) of the polymer film. The decision variables used were the temperature of the isothermal PFTR, concentration of the initiator in the feed to the PFTR, monomer conversion at the end of PFTR, film thickness (all *scalars*), and the temperature programming, $T_w(z)$, in the furnace (a continuous *function*). In order to simplify the problem, the temperature of the surface of the film,

$T_w(z)$, was assumed to be a cubic function of z. Thus, the continuous function was replaced by four constants. The local constraint was taken care of by using the penalty killing procedure. In this study, the requirement, $\mu_{n,av,f} = \mu_{n,d}$, was taken care of by using it *both* as a penalty function in the two objective functions, and also by using it as a stopping condition. This leads to faster convergence to the Pareto solution.

2.8 Other Techniques

Several other workers have used algorithms developed by them or adapted for their particular work to solve multiobjective optimization problems, which cannot be grouped into the above classifications. These are described here. Nishitani and Kunugita (1979) developed a code to determine the optimal flow pattern for multiple effect evaporator systems using a multiobjective approach. A modified parametric method is used in this work. All the objective functions are first represented in terms of a common scale. The problem is split into four simpler problems and solved. Pareto sets are generated between the energy consumption (steam consumption) and an economic objective (heat transfer area). The relationship between the solutions to the four simpler problems and the overall solution to the problem are discussed. Results are obtained for a process for concentrating milk. The conflict between the objectives is not quantitatively understood by this technique, though it is easy to implement for simple systems.

A process design problem was solved by Umeda et al. (1980) using the simplex method (Beveridge and Schechter, 1970; Edgar and Himmelblau, 1988), a pattern search technique, interactively. The pattern search algorithm helps in adjusting the weights of the objectives to find the preferred solution. The proposed method starts with a set of Pareto optimal solutions obtained using a combination of the parametric method and goal programming

(the goal being the utopia point). Then, a more preferred Pareto optimal solution is generated than the existing non-inferior set using the simplex method. Sorting of the members of the subset is done by minimum pair-wise comparison in every iteration. Merging of the new solution with the ordered sub-set is done by the minimum comparison merging technique. Optimal design of a toluene-steam dealkylation process is performed to illustrate the usefulness of the procedure. The objectives considered were (i) the investment cost, (ii) the annual operating cost, and (iii) the reliability of the process. The major advantage of this procedure is that the decision maker (DM) has to put the *current* set of solutions into an order. The method requires the utopia to be determined before the multiobjective optimization problem can be solved.

Takama and Umeda (1980) extended this approach for locating the non-inferior points by decomposing the original (upper-level or interior) problem into simpler (lower-level) sub-problems involving single objective functions. The algorithm generates alternative solutions by solving the sub-problems at lower levels, and performs a search to identify the best compromise solutions from among the alternatives. The DM adjusts the coupling variables at the upper-level and passes the values to each of the lower-level optimization problems, that are then solved. The process is repeated until the DM is satisfied with the solution. The choice of the coupling variables could pose problems because there is no guarantee that all the sub- problems will remain feasible for any set of values of the coupling variables. In addition, it is not necessary that all engineering problems can be decomposed. The authors have applied this algorithm to the optimal design of a water treatment system.

Lenhoff and Morari (1982) proposed a design approach which considers the economic as well as the dynamic aspects simultaneously in the design of resilient processing plants. They used a bounding technique based on the Lagrangian theory, taking advantage of the typical modular structure of processing units. They defined two performance indices: an economic performance index (EPI) and a dynamic performance index (DPI), to characterize a problem. Both of these were minimized and a Pareto set (called the performance index diagram) between the EPI and the DPI was obtained for a sample problem involving three configurations of a heat-integrated distillation column for the methanol-water system. Certain configurations could be eliminated since these were inferior solutions. The effect of changing the steady state design on the performance indices was studied using the bounding technique. A trade-off was found to exist between them, and three non-inferior designs were determined.

Clark and Westerberg (1983) reviewed the mathematical tools used for multi-criteria decision making while addressing problems in design optimization where an 'outer' optimization problem is constrained by an 'inner' one (embedded optimization). They proposed a single level solution to locate the *local optimum* quickly. Two approaches to solve this problem were suggested. The first was based on the active set strategy for solving the inner problem, while the second involved the relaxation of complimentary conditions. The concept of embedded optimization was illustrated on the calculation of the equilibrium composition for multiphase, reacting systems.

An interactive CAD tool, CONSOLE, was used by Butala et al. (1988) for the multiobjective optimization of a semi-batch reactor for the manufacture of styrene-acrylonitrile (SAN) copolymer. Dynamic optimization was used to obtain the two decision

variables, the temperature and the monomer feed rate histories, to produce copolymer having specified values of the average copolymer composition and the average molecular weight. A third-order polynomial was assumed for the two decision variables and their coefficients were obtained using the feasible direction algorithm of Nye and Tits (1986). The problem specifications (both functions and numbers) were classified into objectives, as well as hard and soft constraints. The initial solution had to satisfy the hard constraints first. The soft constraints and the objectives compete simultaneously in the second phase of optimization. In the final phase, the objectives were improved till the DM is satisfied. This process was achieved by scaling of the specification space (GOOD/BAD) based on the DM's knowledge of the process. It is to be mentioned here that this process is highly intuitive and the DM should have a very good knowledge about the problem, before he starts to solve it. Choi and Butala (1991) extended this work to develop open loop optimal control for a semi-batch methyl methacrylate-vinyl acetate (MMA-VA) co-polymerization reactor. The feed rates of the monomers and the temperature of the reactor (both functions of time) were used as decision variables. Copolymer having specified values of the average composition and molecular weight was to be produced. The optimal control policies were tested on an experimental stirred tank polymerization reactor. These workers experienced some plant-model mismatch. The need for improving the optimization method to minimize the plant-model mismatch was indicated.

Ciric and Huchette (1993) tried to minimize the waste treatment costs and maximize the profits of a chemical process, by employing the basic relationship between the sensitivity problem and a multiobjective optimization problem. The proposed approach uses a modified form of the outer approximation method to identify discretely different regions of

the Pareto set. The complete solution set is generated using a sequential approximation algorithm (Ciric and Jia, 1992). The proposed algorithm was applied to the production of ethylene glycol from ethylene oxide and water. This approach is better than the conventional sensitivity analysis techniques such as linear sensitivity analysis and exhaustive search.

Liu et al. (1997) applied the concepts of multiobjective optimization to the multimodel-based minimum bias control of a benchmark paper machine process. They used modified goal programming for solving the problem.

Köllner et al. (1989 a, b) determined the optimal process flow structure for the chlorination of benzene. They used the modified simplex method (Nelder and Mead; Box complex method; Beveridge and Schechter, 1970; Edgar and Himmelblau, 1988) incorporating the inequality constraints on the decision variables, with a stochastic global-search method (Schammler, 1988). They obtained compromise solutions between the total investment cost and variable costs per annum for the optimal process flow structure. They could eliminate four heat exchangers in the process using their study involving multiobjective optimization.

Dimkou and Papalexandri (1998) proposed a decomposition-based algorithm for solving convex MINLP (mixed integer non-linear programming) problems and identifying the Pareto sets. Parametric nonlinear optimization is used to identify the upper bounds of the optimal parametric solution. Lagrangian information from the deterministic non-linear programming (NLP) problems is used to determine the lower bounds to the solution, as is done in Benders' decomposition method (Geoffrion, 1972). The algorithm is illustrated

using two simple examples. The assumption of convexity limits the applicability of the proposed algorithm for real life problems.

Tijsen et al. (1999) generated Pareto sets for the factors affecting the degree of substitution of the hydroxyl groups in starch by ether groups, using experimental data. They optimized the process conditions for the modification of starch. They found the important factors by a backward elimination strategy (Kleinbaum, 1994).

Methods used for generating non-inferior solutions and their applications in Chemical Engineering have been discussed. This forms the objective phase of the decision-making process. A few methods are available to select the best (or preferred) solution from among the Pareto optimal points, using additional, and often non-quantifiable, information. This forms the second, subjective phase. In addition to the technique presented earlier, involving consultation with several DMs to obtain their rankings of the Pareto solutions, the surrogate worth trade-off method (Haimes and Hall, 1974) seems to be popular in Chemical Engineering (Nishitani et al., 1980; Wajge and Gupta, 1994a; Sareen and Gupta, 1995). This method uses the Lagrangian multipliers obtained while generating the Pareto sets, to analyze the trade-offs between the non-commensurate objectives. The preferred solution is usually the one at which the improvement in one of the objective functions is equivalent to the degradation that results in the other objectives.

3. FUTURE DIRECTIONS

Several approaches have been used to obtain solutions of multiobjective optimization problems in Chemical Engineering. It appears that the evolutionary algorithms (e.g., GA, NSGA) used in recent years are quite robust for generating non-inferior solutions for large-

scale complex problems, and will, we expect, become even more popular in the future. These offer several advantages as described below (Deb, 1999):

- Earlier methods have to be applied several times over to (hopefully) obtain a Pareto-optimal solution.
- Some of the methods are sensitive to the shape of the Pareto-optimal front.
- The efficiency of the scalar objective optimization method determines the spread of the Pareto-optimal solutions.
- Uncertainties and stochasticities cannot be handled efficiently using classical methods.
- Problems with a discrete search space cannot be handled efficiently using classical single objective optimization methods (Deb, 1995).

Though NSGA has been tested on several, reasonably large optimization problems in Chemical Engineering, it needs improvement in the area of constraint-handling for still larger and more complex problems. The equality constraints have been handled using the penalty function technique, while the inequality constraints have used penalty killing. In case of problems involving a very large number of constraints, the latter may not be too efficient since there exists a possibility of losing diversity in the gene pool. A better understanding of the values of the computational parameters used in GA and their effects is required to increase their speed of convergence. These have limited the use of NSGA to problems that are not as complex as otherwise possible.

Simulated annealing (SA) is another emerging non-traditional algorithm (Kirpatrick et al., 1983; Aarts and Korst, 1989) which has been used in solving optimization problems in engineering in the recent years, and we expect, will become popular as newer developments

take place. SA mimics the cooling of molten metals in its search procedure. The procedure begins with the selection of an initial solution (called as a point). A neighbouring point is then created and compared with the current point. The algorithm of Metropolis et al. (1953) is used to determine whether the new point is accepted or not. This technique, thus, works with a single point at a time, and a new point is created at each iteration according to the Boltzmann probability distribution. The method is found to be effective in finding global optimum solutions when a slow cooling procedure is used (Deb, 1995). Adaptations can be made in SA to solve multiobjective optimization problems using the concept of non-dominance, somewhat along the lines of NSGA. We expect these adaptations to compete with NSGA in terms of speed of convergence and robustness.

In the next several years, even more complex problems in which the constraints are not known in a very *precise* manner (as discussed in this review), will be solved. In fact, one could easily envisage a situation where a DM looks at two Pareto sets simultaneously, a Pareto between the objective functions, and another Pareto between the *extents* of constraint-violation, to decide upon the preferred solution. Obviously, NSGA will need adaptations to solve such problems, by classifying chromosomes into finer sub-fronts. The only conclusion we can make is that the future holds exciting promises.

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NOMENCLATURE

Symbol	Description
$[C_2]$	Cyclic dimer concentration in nylon 6 manufacture, mol/kg
d_{ij}	Dimensionless distance between the ith and jth chromosomes in the **x**-space
DP	Degree of polymerization ($= \mu_n$)
$F_{CH4,in}$	Flow rate of methane in the input stream, kg/hr
$F_{CO,out}$	Flow rate of CO in the exit stream of the first reactor in the reformer plant (in the syngas), kg/hr
$F_{H2,unit}$	Flow rate of H_2 in the exit stream from the reformer plant, kg/hr
g(x)	Vector of inequality constraints, $g_i(\mathbf{x})$
h(x)	Vector of equality constraints, $h_i(\mathbf{x})$
I	Vector of objective functions, I_i
k_1, k_2	Rate constants in Eq. 2
N_g	Generation number in GA
N_p	Number of chromosomes in the population in GA
p	Pressure
Δp	Pressure drop in cyclone, Pa
Q	Polydispersity index of polymer
Sh	Sharing function (Eq. 10)
t	Time

T	Temperature
u(**I**)	Utility function
V_T	Rate of release of vapor mixture from nylon 6 reactor through control valve, mol/hr
w	Vector of weightage factors, w_i
x_m	Monomer conversion
x	Vector of decision variables, x_i
X	Feasible region of **x**
y	Vector of goals, y_i
z	Axial position in furnace reactor

Subscripts / Superscripts

av	Cross-section average value
d	Desired or design value
f, out	Final, outlet value
J	Jacket-fluid value
ref	Reference value (currentlyused in industrial reactor)
T	Transpose
w	Wall or surface value

Greek

ε_i	Constants in ε-constraint method
η_o	Overall collection efficiency in cyclone
μ_n	Number average chain length of polymer
σ_{share}	Computational parameter in Eq. 10

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TABLE 1: MULTIOBJECTIVE OPTIMIZATION IN CHEMICAL ENGINEERING: BASED ON AREAS IN CHEMICAL ENGINEERING

PROBLEM DESCRIPTION	CONTRIBUTORS
PROCESS DESIGN AND CONTROL	
Multicriteria optimization in chemical processes	Seinfeld and MacBride, 1970
Optimal process systems synthesis	Nishida et al., 1974
Multiple effect evaporator design	Nishitani et al., 1979
Aeration vessel for waste water treatment	Nishitani et al., 1980
Optimal synthesis of methanation process	Shieh and Fan, 1980
Toluene –steam dealkylation process	Umeda et al., 1980
Modeling petrochemical industry	Sophos et al., 1980
Energy resource conservation –Evaporator system	Nishitani et al., 1981
Process design with dynamic aspects	Lenhoff and Morari, 1982
Chemical complexes	Grossmann et al., 1982
Design of chemical plants with robust dynamic operability characteristics	Palazoglu and Arkun, 1986
Complex chemical process system: Benzene chlorination process	Köllner et al., 1989
Modular multivariable controller	Meadowcraft et al., 1992
Binary distillation synthesis	Luyben and Floudas, 1994a
Reactor-separator-recycle system	Luyben and Floudas, 1994b
Minimum bias control of a paper machine process	Liu et al., 1997

POLYMERIZATION REACTION ENGINEERING	
Multiobjective dynamic optimization of semibatch copolymerization reactors/process.	Tsoukas et al., 1982, Butala et al., 1988, Choi and Butala, 1991
Optimization of chain propagation with monomer termination in a batch reactor	Fan et al., 1984
Steady state optimization of continuous co-polymerization reactors	Farber, 1986
Dynamic optimization of a Nonvaporizing nylon 6 batch reactor	Wajge and Gupta, 1994
Optimization of an industrial semibatch nylon 6 batch reactor	Sareen and Gupta, 1995
Dynamic optimization of an industrial nylon 6 semibatch reactor using genetic algorithm	Mitra et al., 1998
Free radical bulk polymerization reactor using genetic algorithm	Garg and Gupta, 1999
Industrial nylon 6 semibatch reactor system using genetic algorithm	Gupta and Gupta, 1999
Industrial wiped film PET finishing reactor	Bhaskar et al., 2000
PMMA reactors and film production	Zhou et al., 2000
BIOCHEMICAL ENGINEERING / WASTE TREATMENT	
Waste water treatment system	Takama and Umeda, 1980
Design and operation of anaerobic digesters using multiobjective optimization criteria	Videla et al., 1990

Fuzzy multiobjective optimization for self-sucking impellers in a bioreactor	Kraslawski et al., 1991b
Waste treatment costs in discrete process synthesis and optimization problems	Ciric and Huchette, 1993
Carboxy-methylation of starch	Tijsen et al., 1999
MIXING	
Kenics static mixers	Kraslawski and Pustelnik, 1991a
CATALYTIC REACTORS	
Steam reformers optimization using GA	Rajesh et al., 2000
ELECTROCHEMICAL PROCESS	
Electrochemical reduction process of maleic-acid to succinic acid	Smigielski et al., 1992
AIR POLLUTION CONTROL	
Cyclone separators	Ravi et al. 2000a
Venturi scrubbers	Ravi et al. 2000b
MEMBRANE SEPARATION MODULES	
Beer dialysis	Chan et al. 2000
GENERAL	
Tools for multicriteria decision making	Clark and Westerberg, 1983
Parametric optimization approach for multiobjective engineering problems involving discrete decisions	Dimkou and Papalexandri, 1998

Table 2

	Contributors	Objective functions	Optimization technique used	Technique used for generation of Pareto set	Technique used for decision making	Remarks
1	Nishitani and Kunugita, 1979	Minimization of energy consumption and minimization of the total cost (capital and operating costs) in a multiple effect evaporator system	A new algorithm developed to generate the non-inferior set of solutions			The algorithm has been applied to milk concentration process.
2	Umeda et al., 1980	Minimization of investment and annual operating costs and Maximization of reliability in a chemical plant	Pattern search algorithm (Simplex method) used to adjust the weights to find the optimal non-inferior solution			A multiobjective optimization algorithm is proposed and applied for a toluene-steam dealkylation process. Method of object weighing is used to scalarize the objective functions
3	Takama and Umeda, 1980	Minimization of the amount of the pollutant discharge and Maximization of the reliability in a waste water treatment unit	Linear search based algorithm which seeks compromise solution by repeating pairwise comparison.			A multilevel, multiobjective optimization algorithm is proposed and applied for a waste water treatment process.The authors claim that the method of trade-off applied in this work is superior than the method of objective weighing in terms of the physical significance of the decision variables.
4	Sophos et al., 1980	Maximization of the thermodynamic availability change, Minimization of the lost work and minimization of the feed stock consumption		ε-constraint approach	Minimization of the deviation from the single objective optimum values with equal weights and the second by commensurating all the objectives and solving a scalar optimization problem	Pareto surfaces determined for three objective function case. Two objective function problem has also been solved.

Table 2 continued

5	Lenhoff and Morari, 1982	Optimal economic and dynamic performance indices among various configurations of binary distillation with heat integration	A new technique, decomposition technique with bounding properties of the Lagrangian was used in the study.			Details of the insight on the trade off policies are exemplified. The interaction between design and control is explained with the help of multiobjective optimization concepts.
6	Tsoukas et al. 1982	Minimization of copolymer composition and molecular weight distributions in styrene-acrylonitrile system	Optimal control theory: Powell's conjugate direction search, algorithm restarted by steepest descent method	ε-constraint approach		Penalty multiplier method used to transform the constrained problem to an unconstrained one. Pareto sets generated.
7	Fan et al., 1984	Minimizing mean and variance of molecular weight distribution of the polymer Maximizing the monomer conversion for a chain propagation polymerization in a batch reactor.		Value function approach and ε-constraint approach		MWD & other criterion functions estimated using numerical solution, continuous variable approximation and discrete exact approach method.
8	Farber, 1986	Methyl methacrylate- Vinyl acetate system 1. Maximization of composition and molecular weight 2. Maximization of conversion and molecular weight Styrene-acrylonitrile system 1. Maximization of conversion and molecular weight	ε-constraint approach			Reactor temperature is the single variable used for MMA-VA system, whereas for SAN system residence time and temperature are considered
9	Palazoglu and Arkun, 1986	Optimum design of the chemical process with robust dynamic operability	Ellipsoid algorithm (modified gradient search technique)	ε-constraint approach		Discretization techniques employed to circumvent the problem of infinite number of constraints in the optimization problem

Table 2 conituned

10	Butala et al., 1988	Minimization in deviation of product specifications from their set values and reaction time.	Nye and Tits technique (1986)		Interaction with the decision maker (DM)	CONSOLE, an interactive optimization based design tool was used. Classification of the constraints done a priori. Optimal open-loop composition & molecular weight control for copolymerization of SAN system.
11	Videla et al., 1990	1.Maximize the net production of energy in terms of biogas 2. Maximize the Percentage COD removal 3.Minimize the capital costs for an anaerobic digester	MINOS IV	ε-constraint approach	Surrogate Trade-offs based on priorities by DM	Optimal solutions generated for minimum cost and maximum net biogas production with at least 75% COD removal. Weights are changed based on the physical significance.
12	Choi and Butala, 1991	Minimization in deviation of product specifications (composition and MWD) from their set values for fixed reaction time.	Nye and Tits technique (1986)		Interaction with the decision maker (DM)	Experimental study, carried out for both isothermal and non-isothermal copolymerization.CONSOLE, an interactive optimization based design tool was used. Classification of the constraints done a priori. Optimal open-loop composition & molecular weight control for copolymerization of MMA-VA system.
13	Kraslawski et al., 1991	Maximization of k_La, the mass transfer parameter for aeration and minimization of the power consumption	Modified Goal Programming			Two level process observed. In the first level, the type of of the mixing equipment was chosen and in the second level, the optimum operating conditions for this type is determined using the fuzzy weights assigned to each of the objective functions.
14	Kraslawski and Pustelnik, 1991	Minimize pressure drop and Maximize the degree of mixing in Kenics static mixer	Min-Max method & Sequentially built compromise function			Assumption of weights is arbitrary for the objective functions and a complete study needs to be done with various other weightage factors.

Table 2 continued

15	Smigielski et al., 1992	Maximization of the degree of inversion from maleic to succinic acid and minimization of the amount of wastes produced in the electrochemical reduction process	Goal Programming			Optimization carried out without using a mathematical model using utopia points and the weights, selected by fuzzy set theory.
16	Ciric and Huchette,1993	Maximize net profits before waste treatment and minimize waste production	Generalized Bender's Decomposition Algorithm for MINLPs	Modified outer approximation technique identifies the non-inferior set and the full curve is identified by Sequential approximation algorithm		Novel approach to identify the Pareto set in a discrete multiobjective optimization problem proposed and applied to the production of ethylene glycol from ethylene oxide and water.
17	Luyben and Floudas, 1994	Total cost (operating and capital costs) / year and the open-loop controllability objectives considered in application to binary distillation synthesis	Generalized Bender's Decomposition Algorithm for MINLPs.MINOS 5.2 (Murtagh and Saunders, 1988)	ε-constraint approach	Cutting Plane Method	Various possible control configurations, objectives and heat integration modes of the binary distillation synthesis considered and a the best compromise solution found using the information on the slope of the Pareto set.
18	Luyben and Floudas, 1994	Steady state economic gain and the open-loop controllability objectives analyzed for reactor-separator-recycle system		ε-constraint approach	Cutting Plane Method	Various possible control configurations and objectives of the system considered.
19	Wajge and Gupta, 1994	Minimization of the 1. Concentration of unreacted monomer in the product 2. Dimer concentration 3. Reaction time for producing nylon 6 of specified average molecular weight.	Pontryagin's minimum principle combined with Lagrange multipliers	ε-constraint approach	Surrogate Worth Trade-off method	Two problems studied with two objective functions at a time. Pareto sets generated for the same and optimal temperature histories generated.

Table 2 continued

20	Sareen and Gupta, 1995	Minimization of the reaction time and the cyclic dimer concentration in an industrial semibatch nylon 6 reactor for three different grades.	Sequential Quadratic Programming (SQP). Hessian update by modified BFGS quasi-Newton method	ε-constraint approach	Surrogate Worth Trade-off method	Equality constraint on the desired number average molecular weight and Stopping condition on the desired conversion imposed. Smoothening of the Pareto sets to yield suboptimal solution sets carried out.
21	Mitra et al., 1998	Minimization of the reaction time and the cyclic dimer concentration in an industrial semibatch nylon 6 reactor.	Nondominated Sorting Genetic Algorithm (NSGA)			Equality constraint on the desired number average molecular weight and Stopping condition on the desired conversion imposed. Adaptation made to give optimal vapor release rate history (continuous variable rather than a discrete point). Also, optimal value of the jacket fluid temperature generated.
22	Garg and Gupta, 1999	Minimization of total reaction time and the polydispersity of the PMMA product	Nondominated Sorting Genetic Algorithm (NSGA)			Endpoint constraints on the number average chain length and the monomer conversion incorporated. Unique optimal solution obtained.
23	Gupta and Gupta, 1999	Minimization of the reaction time and the cyclic dimer concentration in an industrial semibatch nylon 6 reactor system.	Nondominated Sorting Genetic Algorithm (NSGA)			Equality constraint on the desired number average molecular weight and Stopping condition on the desired conversion imposed. Optimal fractional control valve opening and the optimal value of the jacket fluid temperature generated.

Table 2 continued

24	Rajesh et al., 2000	Minimization of the methane feed rate and maximization of the flowrate of CO in the syngas for a fixed production rate of hydrogen in an existing side-fired steam reformer	Nondominated Sorting Genetic Algorithm (NSGA)		Mapping of the decision variable values done inside the NSGA code to make the bounds chromosome specific(depending on the choice of other decision variables).
25	Bhaskar et al., 2000	Minimization of the residence time of the polymer melt and the concentrations of the undesirable side products formed in the industrial continuous wiped film PET reactor.Equality constraint on the desired degree of polymerization imposed.	Nondominated Sorting Genetic Algorithm (NSGA)		NSGA adapted to use inequality constraints on certain product properties by "artificial killing" of the chromosomes in the process of optimization. Unique optimal solution obtained.
26	Ravi et al., 2000	Maximization of the overall collection efficiency and minimization of the pressure drop / overall cost of the cyclone separators	Nondominated Sorting Genetic Algorithm (NSGA)		Additional bounds and over-riding constraints needed to be imposed. Bounds were made chromosome specific.
27	Chan et al., 2000	Maximization of the percentage removal of the alcohol from beer and minimization of the removal of the 'extract' (taste chemicals)	Nondominated Sorting Genetic Algorithm (NSGA)		Procedure to develop useful design charts representing trade-offs developed and few other optimization problems studied.
28	Zhou et al., 2000	Maximization of the monomer conversion (cross-section average value) and minimization of the length of the film reactor in the continuous casting process for PMMA	Nondominated Sorting Genetic Algorithm (NSGA)		Constraints on the number average molecular weight and the temperature imposed.

Figure 1

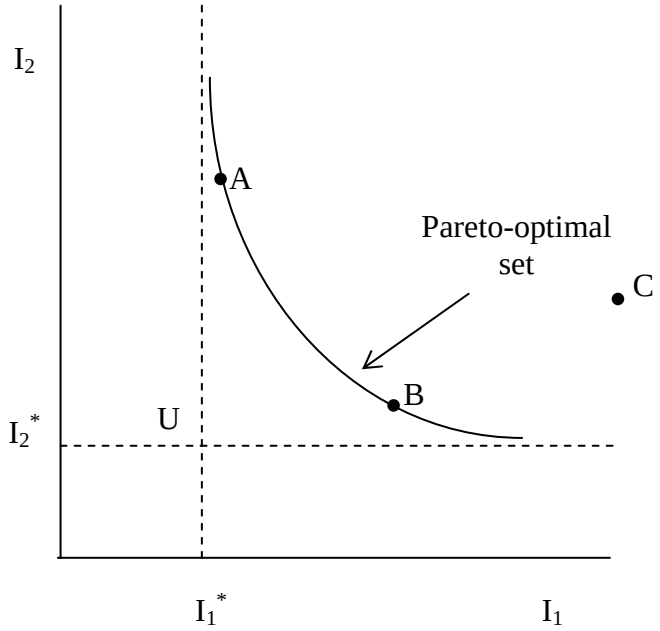
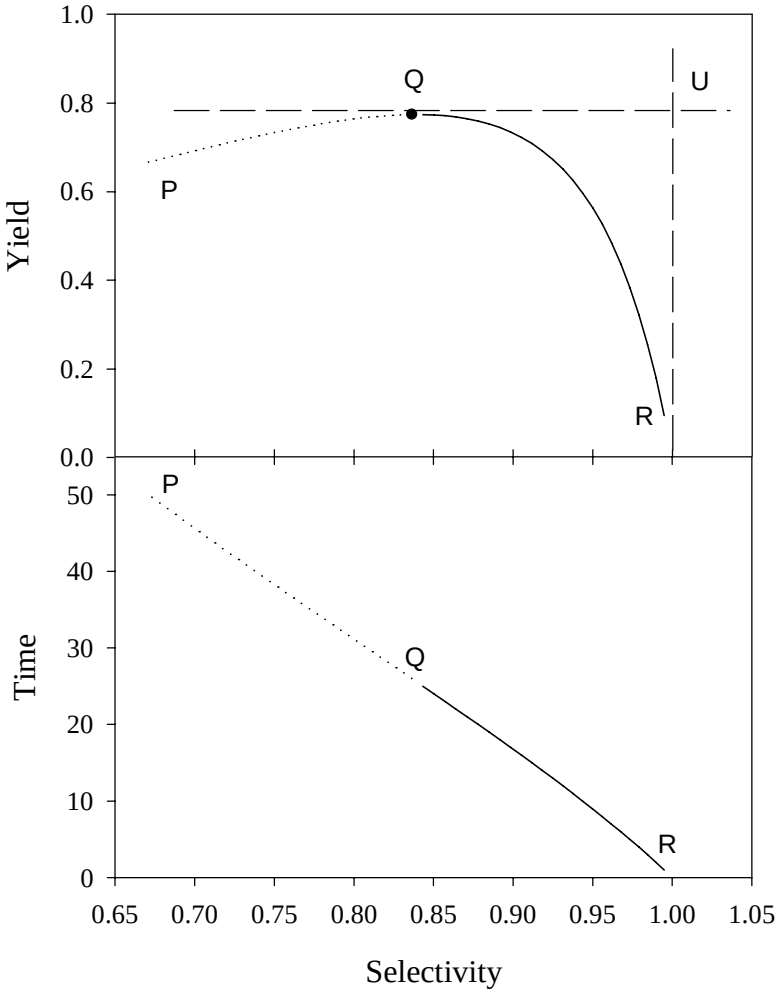


Figure 2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Time
P
Q
R
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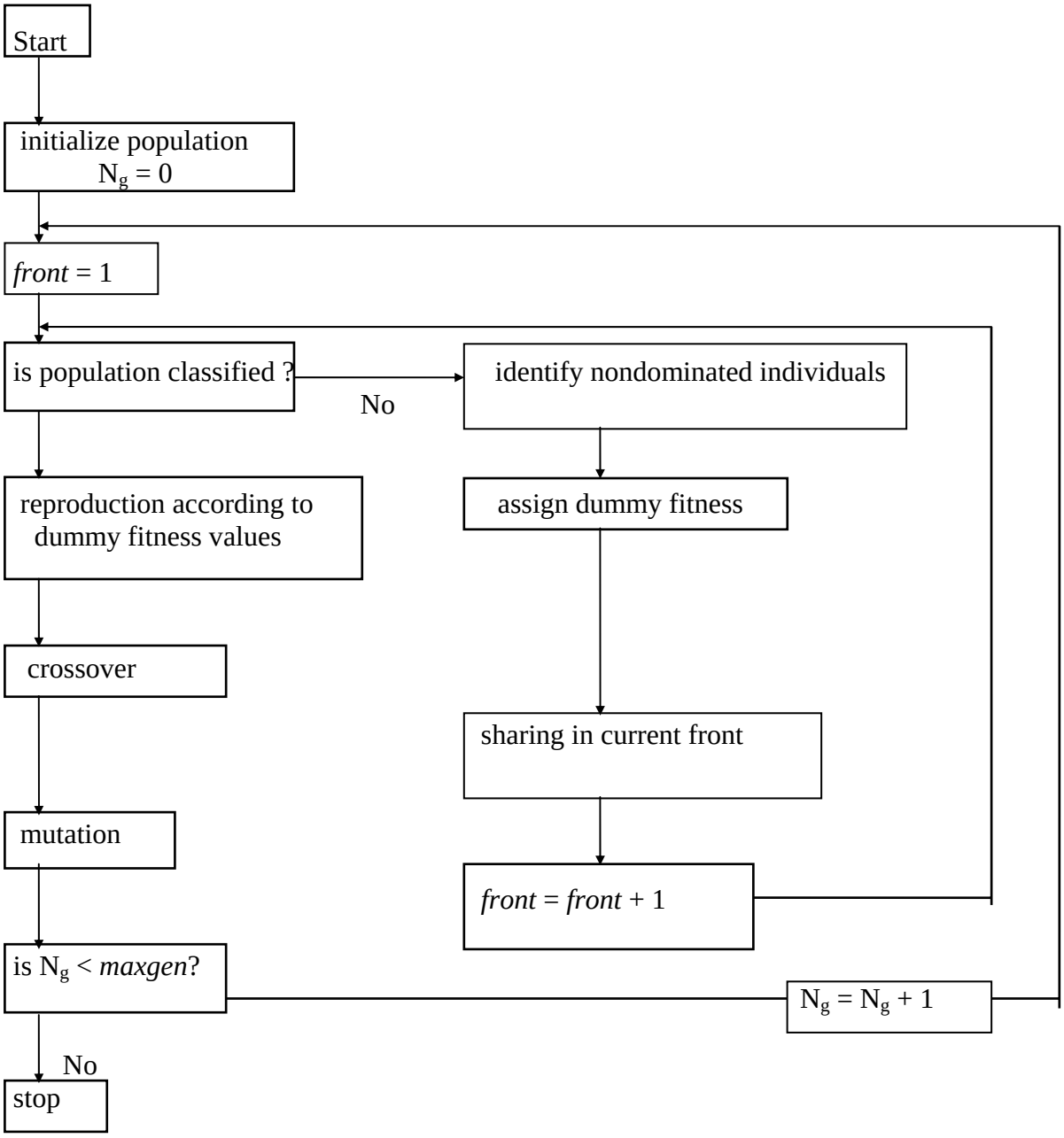
Selectivity

Figure 3

FLOWCHART OF NSGA



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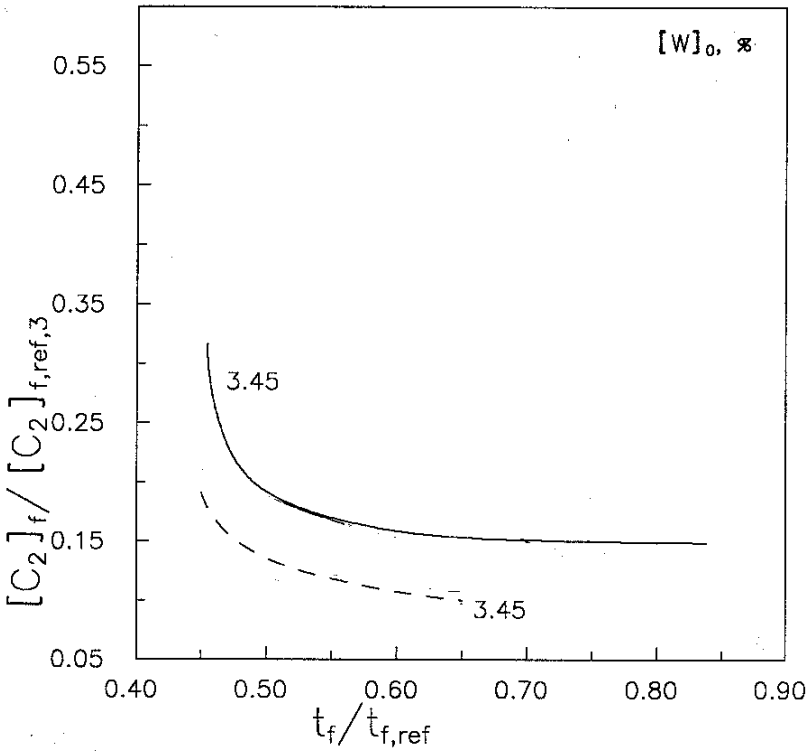
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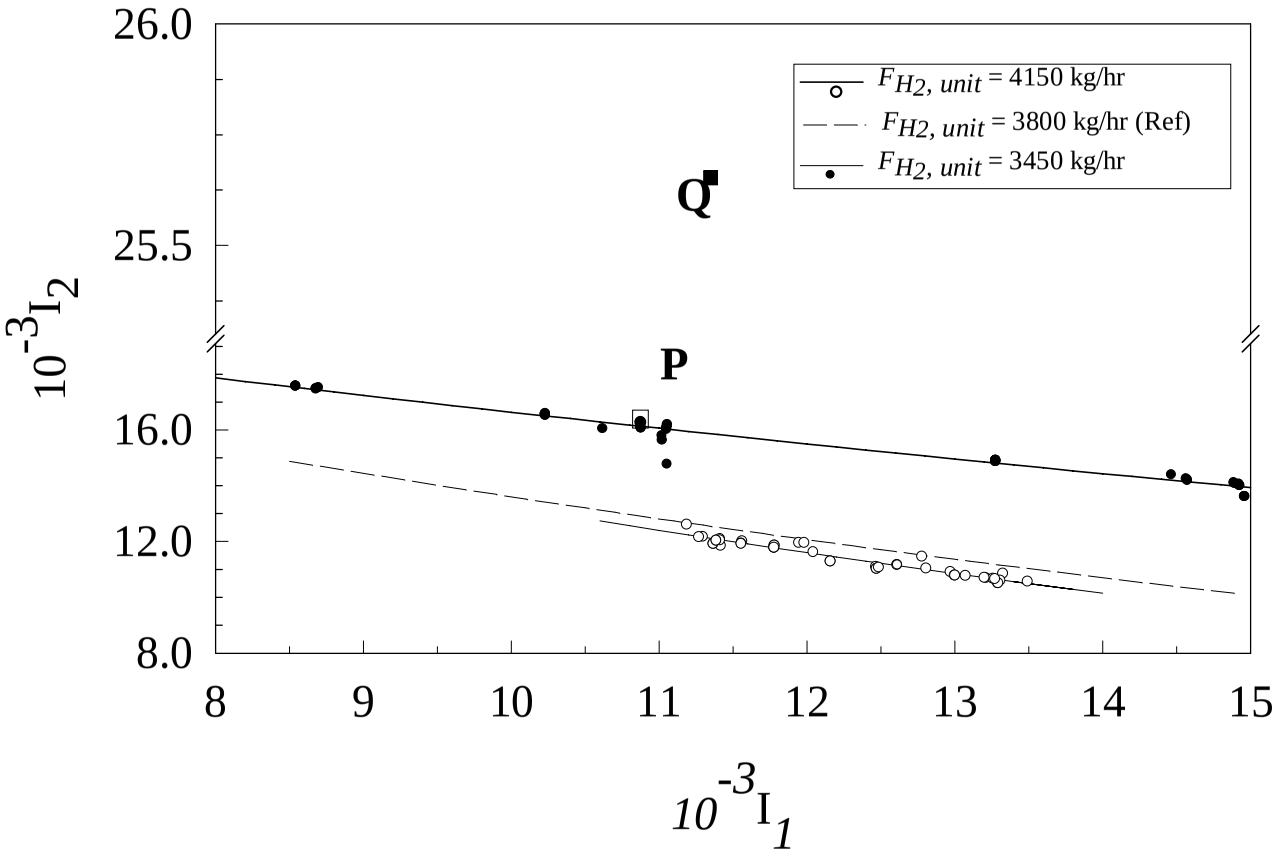
Figure 5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$10^{-3}I_2$
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$F_{H2,\ unit}$ = 4150 kg/hr
$F_{H2,\ unit}$ = 3800 kg/hr (Ref)
$F_{H2,\ unit}$ = 3450 kg/hr
Q
P

Figure 6