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Applications of the Non-Dominated Sorting Genetic Algorithm (NSGA) in Chemical Reaction Engineering

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Applications of the Non-Dominated Sorting Genetic Algorithm (NSGA) in Chemical Reaction Engineering

Anjana D. Nandasana, Ajay Kumar Ray, and Santosh K. Gupta

Abstract

Most of the chemical reaction engineering optimization problems encounters more than one objective functions. A considerable amount of research has been reported on the multiobjective optimization of various chemical reactors using various non-dominated sorting genetic algorithms. This is reviewed in this paper. The introduction of the topic is given at the beginning, followed by the description of multi-objective optimization and Pareto set. We have then discussed various non-dominated sorting genetic algorithms and its applications in chemical reaction engineering. Some comments are also made on the future research direction in this area.

KEYWORDS: Multiobjective optimization, Pareto, Reactors, Modeling, Simulation

1. INTRODUCTION

Chemical engineering is associated with core competencies in several major areas. These include reaction engineering, transport phenomena, separations science and computational and systems science. Chemical reaction engineering plays a vital role in chemical engineering processes. Even though the cost of the reactors may not be a significant fraction of the total plant cost, the downstream separation costs depend to quite an extent on the composition of the reactor effluent, and the economics of the entire plant often depends on the efficient operation of the reactor. The modeling, optimization and control of reactors is, thus, quite important.

A considerable body of literature already exists on the modeling of reactors, and several complex reactors of industrial relevance have been modeled and tuned against plant data. The optimization of complex industrial reactors has started receiving attention only in the last one or two decades. In searching for the optimum, the cost of the reactor obviously needs to be minimized. However, additional important aspects need to be optimized simultaneously, e.g., process and product safety, minimization of waste generation, operability, control, etc. Indeed, most of the problems in chemical reaction engineering involve the optimization of *several* objective functions (multiobjective optimization) simultaneously. This forms the focus of the present paper.

Different optimization techniques have been used to solve problems of chemical engineering interest ever since the late 1940s. Several excellent texts (Beveridge and Schechter, 1970; Bryson and Ho, 1969; Deb, 1995; Edgar and Himmelblau, 2001; Gill et al., 1981; Lapidus and Luus, 1967; Ray and Szekely, 1973; Reklaitis et al., 1983; Wilde, 1964) describe these techniques, and provide relatively *simple* examples. In the last decade, the focus has shifted to the multiobjective optimization of complex *industrial* systems, using a variety of mathematical techniques and robust computational algorithms. The non-dominated sorting genetic algorithm (NSGA) and its adaptations have become popular for solving such problems. This short review describes these techniques and discusses their recent applications in the area of chemical reaction engineering. Some conjectures at a conceptual level are presented thereafter.

2. MULTIOBJECTIVE OPTIMIZATION

Until about 1980, virtually all problems in chemical engineering were optimized using *single* objective functions. Often, the objective function (also called the cost function) involved the economic efficiency, a scalar quantity. Most real-world chemical reaction engineering problems require the simultaneous optimization of *several* objectives (multiobjective optimization) that are non-commensurate, and so cannot be combined into a single, meaningful scalar objective function. 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 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 that there is a risk of losing some optimal solutions (Chankong and Haimes, 1983; Haimes, 1977). The desirability function approach (Derringer, 1980; Deming, 1991) is another most widely used methods in industry for the optimization of multiple response processes. It is based on the idea that the "quality" of a product or process that has multiple quality characteristics, with one of them outside of some "desired" limits, is completely unacceptable. The method finds operating conditions that provide the "most desirable" response values. Harrington first introduced the concept (Harrington, 1965).

The concept of multiobjective optimization is attributed to the economist, Pareto (1896). This has become popular in engineering recently. Here, we focus on the multiobjective optimization of reactor systems only. To the best of our knowledge, the first published studies on multiobjective optimization in chemical reaction engineering are those on copolymerization reactors (Butala et al., 1988; Fan et al., 1984; Farber, 1986; Tsoukas et al., 1982).

3. PARETO SET

A multiobjective optimization problem consists of several objective functions that are either to be minimized or maximized. A number of constraints need to be satisfied simultaneously. A typical two-objective function minimization problem can, thus, be represented mathematically as

$$\text{Min } \mathbf{I}(\mathbf{x}) \equiv [I_1(\mathbf{x}), I_2(\mathbf{x})] \quad (1a)$$

subject to (s.t.):

$$\text{Model equations;} \quad (1b)$$

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

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

In Eq. 1, $\mathbf{x}$ represents a p -dimensional vector of p design or *decision* variables. It is found that the (feasible) solution of Eq. 1 often (but *not* always) comprises of *several* optimal solutions, $\mathbf{x}$, and is not necessarily a unique, single point. These solutions correspond to different values of I_1 and I_2 . Figure 1 shows the optimal solutions of Eq. 1 schematically. Each point in the I_2 vs. I_1 plot in Figure 1 corresponds to an optimal solution, $\mathbf{x} (\equiv [x_1, x_2, \dots, x_p])$, of Eq. 1. The curve in Figure 1 is referred to as a Pareto set (Chankong and Haimes, 1983). If we consider two points, A and B, on this set, we find that on moving from one to the other, one objective function improves (decreases) while the other one worsens (increases). These points are equally good (non-dominating or non-inferior). More formally and generally, non-inferior points are those for which, on moving from one point to the other, an improvement in any one objective function cannot be obtained without deterioration in *at least* one of the other objectives. Points A and C are non-dominating but C is an inferior point since B is superior to it. Graphical representation of the Pareto points for three or more objectives is quite cumbersome (see Deb, 2001; Nayak and Gupta, 2003, for methods to study these).

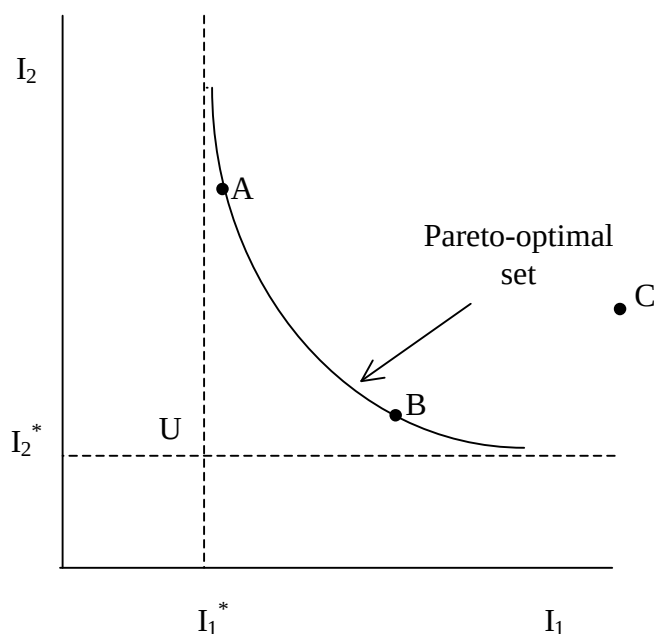


Figure 1. Diagram of Pareto optimal set for a two objective function optimization problem.

Generating the Pareto set comprises the first or objective phase of a multiobjective optimization study and narrows down the choices available to a decision-maker (DM). 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* $I_i(\mathbf{x})$. 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), but represents a useful reference or ideal point. 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. Most available codes (e.g., Deb, 1995, 2001) maximize *all* the objective functions. In case one

needs to minimize any objective function, I_i , one replaces it by the maximization of a *fitness function*, F_i . A popular transformation is $F_i \equiv 1/(1 + I_i)$.

The second, subjective phase involves the selection of the *preferred* solution from among the Pareto points. One method is to have several decision makers (DMs) rank the Pareto solutions using their judgement, and the preferred solution, thus, decided upon. Alternatively, the surrogate worth trade-off method (Haimes and Hall, 1974) seems to be popular in chemical engineering (Nishitani et al., 1980; Sareen and Gupta, 1995; Wajge and Gupta, 1994) to obtain this preferred solution. 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.

4. ALGORITHMS FOR MULTIOBJECTIVE OPTIMIZATION

Extensive research has been reported on the algorithms used for generating the non-inferior Pareto solutions. These are described in several textbooks (Carlos et al., 2002; Chankong and Haimes, 1983; Cohon, 1978; Deb 2001; Goicoechea et al., 1982; Haimes and Hall, 1974; Haimes et al., 1990; Hwang and Masud, 1979; Steuer, 1986; Zeleny, 1974, 1982) and research and review articles (Geoffrion, 1967a-c; Geoffrion et al., 1972, Hwang et al., 1980; Srinivas and Deb, 1995; Zionts and Wallenius, 1976, 1980). The algorithms include: vector-evaluated GA (VEGA; Schaffer, 1984), vector-optimized evolution strategy (VOES; Kursawe, 1990), weight-based GA (Hajela et al., 1992), multiple-objective GA (Fonseca and Fleming, 1993), niched Pareto GA (Horn and Nafploitis, 1993), distance-based Pareto GA (Osyczka and Kundu, 1995), non-dominated sorting GA (NSGA-I; Srinivas and Deb, 1995), thermodynamical GA (Kita et al., 1996), random-weighted GA (Murata, 1997), strength Pareto evolutionary algorithm (SPEA; Zitzler and Thiele, 1998), multiobjective messy GA (van Veldhuizen, 1999), Pareto-archived evolution strategy (PAES; Knowles and Corne, 2000), NSGA-II (Deb et al., 2002) and NSGA-II-JG (Kasat and Gupta, 2003). These have been extensively reviewed in the recent books of Deb (2001) and Carlos et al. (2002), and the advantages and disadvantages of the different algorithms have been pointed out, using *simple* examples. In the present work, we focus attention only on the applications of NSGA and its two adaptations, NSGA-II and NSGA-II-JG, since these have been used extensively in chemical reaction engineering.

4.1 NSGA-I AND ITS APPLICATIONS

In this section, we first describe NSGA-I (Srinivas and Deb, 1995). This algorithm builds upon the basic framework provided by Holland (1975). In NSGA-I, an initial population of several *chromosomes* is generated randomly. A chromosome (or gene) is a string of numbers (often binaries), coding information about the decision variables. The subsets (substrings) in any chromosome associated with the different decision variables, are then *mapped* into real and meaningful values lying between the corresponding specified bounds. A model for the process (reactor) is then used to evaluate the values of the fitness functions. A set of the good non-dominated chromosomes are identified. This is done by testing each of the chromosomes in the population against *all* others (pair-wise comparison, involving a large number of computational steps). As soon as a chromosome is found to be dominated, it is not checked for dominance any further. After testing all the chromosomes in this manner, we are left with a sub-set of the *best* non-dominated chromosomes. This is assigned a front number of unity (Front No. = 1). The remaining solutions are again compared as before, and the next set of non-dominated solutions is identified and assigned a Front No. of 2. This procedure is repeated. Clearly, fronts having lower values of the front number are superior or non-dominated sets when compared to those having a higher front number. A high *fitness value* (assigned single, common value) is assigned arbitrarily to *all* the solutions of Front No. 1. The fitness values of individual chromosomes in this front are then modified based on their “degree of crowding”. This is estimated using information on the distance between pairs of chromosomes, either in the *x*-space or in the *F*-space. A niche count (= number of “nearest” neighbours) is evaluated for *each* chromosome in Front No. 1. One could define a fixed neighbourhood for a chromosome and count the neighbours lying in it. Alternatively, we could use a suitable decreasing function (sharing function) of the distance from a reference chromosome to evaluate this niche count of “nearest” neighbours. In this latter approach, a neighbour that is farther contributes less to the niche count than one that is closer to the reference chromosome. The common fitness value assigned earlier to all the members of this front, is divided by the niche-count of any chromosome to evaluate its *shared* fitness value. The common fitness value assigned to *all* members of Front No. 2 should, obviously, be smaller (arbitrarily again) than the lowest shared fitness value in Front No. 1. This procedure is continued till all the chromosomes in the population have been

assigned shared fitness values. The use of this procedure enables the spreading out of the chromosomes. This step is followed by reproduction. The chromosomes are copied stochastically (best chromosome having a higher probability) into a mating pool. There are numerous selection techniques, e.g., roulette wheel, tournament selection (popular), normalized geometric ranking, expected value and linear normalization (Deb, 2001). This copying procedure exploits the Darwinian principle of survival of the fittest.

Crossover and mutation are now performed on these copies to give daughter chromosomes (and complete a generation). In crossover, chromosome information is exchanged between two individuals randomly selected from the mating pool. For example, a pair of binary coded chromosomes, 101001 and 010110, after crossover at the third (randomly selected) location, will give two chromosomes, 101110 and 010001. In mutation, each binary number in every single chromosome is changed with a specified mutation probability, using a random number code. The mutation probability is small so as to avoid oscillatory behaviour. The above procedure is repeated several times (generations) until a satisfactory set of Pareto optimal solutions are obtained in the gene-pool, having a reasonable spread of points. The flowchart of NSGA-I is available in Mitra et al. (1995). User-friendly codes of NSGA-I are available at <http://www.iitk.ac.in/kangal>.

NSGA-I has been applied extensively in chemical engineering. These have been reviewed recently by Bhaskar et al. (2000a). In this paper, however, only those applications that relate to reactors are presented (and updated). The first application of NSGA-I in chemical reaction engineering was for an industrial nylon 6 semi-batch reactor (Mitra et al., 1998). In fact, this work was the first to extend NSGA-I (Srinivas and Deb, 1995) to multiobjective optimization problems involving variables that are *continuous functions*. The two objective functions used were to minimize (i) the total reaction time, t_f (subscript, f, indicates final), and (ii) the concentration, $[C_2]_f$, of the undesirable cyclic dimer (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 as to obtain product having the design values, $x_{m,d}$ and $\mu_{n,d}$, respectively. 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) that influences the pressure history, $p(t)$, in the reactor, and (ii) the jacket fluid temperature, T_J (a scalar). The continuous function, $V_T(t)$, was discretized into several, equi-spaced (in time) scalar values, $V_{T,i}$; $i = 1, 2, \dots, Q$, and the value of $V_{T,i}$ was constrained to lie (randomly) within a small range of the *previous* value, $V_{T,i-1}$, i.e., the permissible range of $V_{T,1}$ was much larger than those of the subsequent $V_{T,i}$. This enabled $V_T(t)$ to be implementable. Pareto-optimal solutions were obtained. Mitra et al. found that the solutions obtained by NSGA-I were superior to these of Sareen and Gupta (1995), who had introduced artificial constraints by parameterizing the decision variables. They used Pontryagin's minimum principle. Interestingly, considerable improvement in the operation of the reactor has been achieved industrially.

Gupta and Gupta (1999) extended this work and considered the fractional opening of the control valve as one of the decision variables (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 worse than those obtained by Mitra et al. because the operation of the control valve excluded some $V_T(t)$. 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-I 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 (PMMA) 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. Optimal temperature histories, $T(t)$, were generated for a given initiator concentration in the feed. Interestingly, a unique optimal solution was obtained 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.

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) used 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, the temperature at *any* point in the film must be below a safe upper 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 the 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 parameterized using cubic functions of z .

Bhaskar et al. (2000b) solved a multiobjective optimization problem for an industrial, third stage wiped-film reactor used to produce polyethylene terephthalate (PET). The objective functions used were to minimize the concentrations of two undesirable side products in the polymer, namely, the acid end group and the vinyl end group. An equality constraint was imposed on the degree of polymerization, DP_{out} , of the product ($DP_{out} = DP_d$). The acid end group concentration in the product was further restricted to lie below a certain value (an inequality constraint), while the concentration of the diethylene glycol end group in the product was restricted to lie in a specified *range* (two inequality constraints), in accordance with industrial practice. The solution of the problem was found to be a unique point. Bhaskar et al. (2001) found that when the temperature was included in the set of decision variables, a unique optimal point was always obtained. In contrast, when the temperature was specified and was not a decision variable, Pareto optimal solutions were obtained. Interestingly, these workers found that the optimal solutions depend on the value used for one of the computational parameters (random seed). Pareto solutions were actually generated using *several computational runs* with different values of the random seed. This represents a failure of NSGA-I.

Rajesh et al. (1999) carried out the multiobjective optimization of an industrial side-fired steam reformer reactor (Elnashaie and Elshishini, 1993, 1996), the first reactor in a steam reforming plant, using NSGA-I. Two objective functions were considered: (i) minimization of the methane feed rate (input to the reformer), $F_{CH_4,in}$, required for a specified rate of production of hydrogen, $F_{H_2,unit}$, 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 first-principles model (tuned on industrial data). The rate of production of hydrogen was equated to a desired value, and an upper cap was imposed on the maximum wall temperature of the reformer tubes. This is crucial since even a 1 K increase in the maximum wall temperature beyond a critical limit of 1200 K of the reformer tube material can lead to a significant (several years) reduction in the working life 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 were obtained. These workers found that several of the randomly generated chromosomes in the early generations, failed to converge. This problem was taken care of by using *chromosome-specific bounds* of the decision variables, these being decided based on experience with simulation runs. Rajesh et al. (2001) subsequently extended this work on the first reactor to the entire hydrogen plant (steam reformer reactor + two shift converters, etc.). Simultaneous maximization of the product hydrogen and export steam flow rates were considered as the two objective functions for a fixed flow rate of methane to the industrial unit. The inequality constraint on the maximum wall temperature was also used. Pareto optimal solutions were obtained. Oh et al. (2001) improved upon this work by adding a third objective function, viz., minimization of the reformer duty. They replaced the flue gas temperature by the heat flux profile as a decision variable. Results obtained were observed to be better than those obtained in the earlier study of Rajesh et al. (2001). Oh et al. (2002a) recently optimized an existing industrial hydrogen plant using refinery off-gas as the feed. The feed stream is a mixture of liquefied petroleum gas and off-gases from a membrane separation unit in a petroleum refinery. For a fixed feed rate of the off-gas to the unit, three objective functions were studied. These were the maximization of the (i) product hydrogen and the (ii) export steam flow rates, and (iii) the minimization of the heat duty supplied to the steam reformer. The optimal heat flux profile in the steam reformer was found to be different from that obtained with methane feed both for operation stage (Oh et al., 2001) and design stage (Oh et al., 2002b) optimization. These workers found that the optimal solutions led to an improvement of the current operation of the industrial unit.

Yee et al. (2003) carried out the multiobjective optimization of two kinds of industrial styrene reactors: (i) an adiabatic and (ii) a steam-injected reactor. Several two- and three-objective functions were considered from

among (a) the production, (b) yield, and (c) the selectivity of styrene. The decision variables used for the adiabatic reactor were: the feed temperature of ethyl benzene, the inlet pressure, the molar ratio of steam to ethyl benzene, and the initial flow rate of ethyl benzene. Two additional decision variables (total of six) were selected for the optimization of the steam-injected reactor. These were the fraction, δ , of steam used at the reactor inlet, and the non-dimensional location, λ , of the injector port for the remaining steam. Three inequality constraints were imposed on the total steam flow rate, the temperature of the ethyl benzene-steam mixture entering the reactor inlet, and the temperature at $z = \lambda L$. For the adiabatic reactor, only the first two constraints were imposed. Pareto optimal solutions were obtained. Later Li et al. (2003) extended the optimization study for an existing styrene reactor to the design stage. They determined optimal diameter and optimal length to diameter and found improved results over existing reactor systems.

Ziyang et al. (2001) optimized a simulated countercurrent moving bed chromatographic reactor (SCMCR) for the synthesis of methyl tertiary butyl ether (MTBE). Three different multiobjective optimization problems having practical relevance were studied in this work, namely, (a) the simultaneous maximization of the purity and the yield of MTBE; (b) the simultaneous maximization of the purity and yield of MTBE, together with the minimization of the total amount of adsorbent/catalyst required; and (c) the maximization of the purity of MTBE with the simultaneous minimization of the eluent consumption. Pareto optimal solutions were obtained in all. Chen et al. (2003) obtained optimal Pareto solution for oxidative coupling of methane to ethane and ethylene in SCMCR. They maximized conversion and selectivity of valuable C_2 (intermediate) products over complete conversion to CO and CO_2 products. Recently, Yu et al. (2003) optimized modified SCMCR systems, namely Varicol process (which is based on non synchronous switching) for synthesis of methyl acetate ester. They reported much improved optimal solution over traditional SCMCR.

4.2 NSGA-II

Experience with NSGA-I indicates that this algorithm has some disadvantages. The sharing function used to evaluate niche count of any chromosome requires the values of two parameters, which are difficult to assign *a-priori*. The total complexity of NSGA-I is MN_p^3 , where M is the number of objective functions, and N_p is the number of chromosomes in the population. In addition, NSGA-I does not use any elite-preserving operator and so, good parents may get lost. Deb et al. (2002) have recently developed an elitist non-dominated sorting genetic algorithm (NSGA-II) to overcome these limitations. We describe below the two major departures of NSGA-II over NSGA-I (see the early part of the flow chart in Fig. 2):

(i) In NSGA-II, the initial N_p parent chromosomes (in box P) are classified into fronts based on non-domination using a different procedure. A new box, P' is created, having size, N_p . A chromosome (starting from the first) in box P is removed and compared with all the solutions already present in box P' . Any chromosome in P' that is dominated over by this latest chromosome under consideration, is removed from P' and put back into its original place in P . If, however, no such chromosome is found, P' is a non-dominated solution, and is kept in P' . This is repeated with all N_p chromosomes in P , sequentially. At the end, the best set of non-dominated chromosomes (a subset of those originally in P) is present in P' . This subset constitutes the first front or sub-box (having size $\leq N_p$) of non-dominated chromosomes, and is assigned a Rank No., I_{rank} , of 1. Subsequent fronts are created as sub-boxes of P' using the chromosomes *remaining* in P . Rank numbers, 2, 3, ..., are assigned to these fronts. In the present procedure, a comparison of the chromosomes is carried out *only* with the members present in the current sub-box. This reduces the numerical complexity of the front-assigning step to MN_p^2 operations.

The chromosomes in each of the fronts in P' are then arranged in ascending order of the values of *any* one of their fitness functions. The largest M -dimensional cuboid (rectangle for two fitness functions) is drawn around any chromosome that just touches its nearest neighbours in the $\mathbf{F}$ -space. The crowding distance, I_{dist} , for this chromosome is taken to be half the sum of all the sides of this cuboid. The boundary solutions in any front are assigned arbitrarily large crowding distances (so as to give them considerable weight).

Two chromosomes are now picked randomly from all the N_p chromosomes in P' , and the better of these two (having a smaller value of I_{rank} or, if I_{rank} are identical, having a larger value of I_{dist}) is copied into a new box, P'' , having N_p positions. This procedure is repeated till P'' has N_p members. Clearly, multiple copies (or no copy) of any chromosome in P' may be present in P'' .

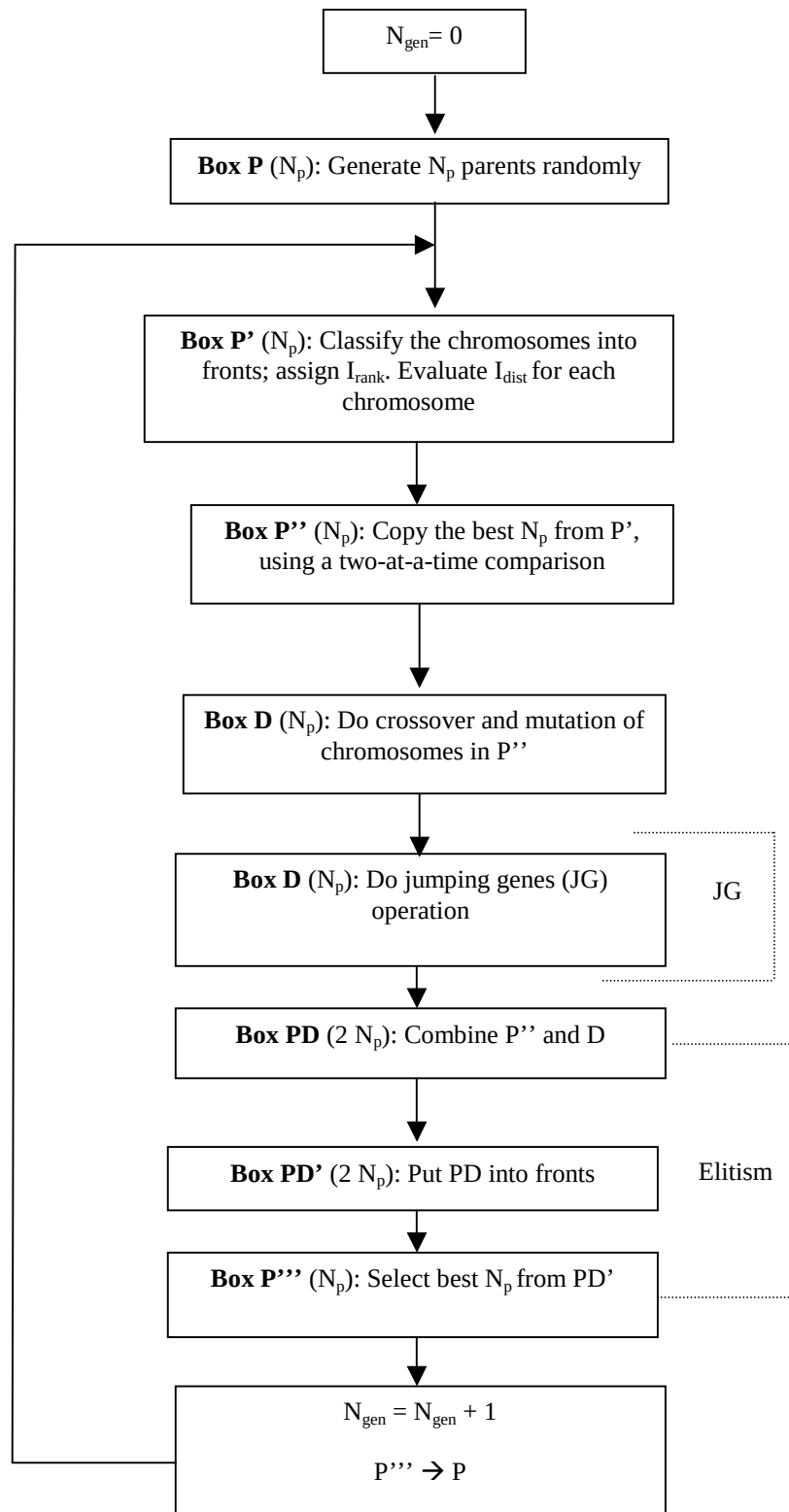


Figure 2. Flow chart for NSGA-II and NSGA-II-JG (Kasat and Gupta, 2003).

Chromosomes in P'' are copied to a new box, D , having N_p locations again. Crossover and mutation are carried out on the chromosomes in D . This gives N_p daughter chromosomes.

In order to ensure elitism (carrying forward the better parents to the next generation), all the N_p best parents (in P'') and all the N_p daughters (in D) are copied into a new box, PD , having size $2N_p$. These chromosomes are reclassified (and placed in PD') using *only* the criterion of non-domination. The best N_p parents are selected and placed in box, P''' . This completes one generation and ensures the elite parents to be present. User-friendly codes of NSGA-II are available at <http://www.iitk.ac.in/kangal>.

Kasat et al. (2002) optimized an industrial fluidized-bed catalytic cracking (FCC) unit to obtain optimal operating conditions. This is a computationally intensive problem, since it involves an iterative solution of the equations describing the two connected reactors: the riser-reactor and the regenerator. NSGA-II was used to solve a three-objective function problem. The objective functions used were: maximization of the gasoline yield, minimization of the air flow rate to the regenerator, and minimization of the per-cent CO in the flue gas coming out of the regenerator. A fixed feed (gas oil) flow rate was used. The decision variables used were: pre-heat temperature of the feed to the riser reactor, air pre-heat temperature, circulation rate of the catalyst, and the flow rate of air. Pareto optimal solutions were obtained. These correspond to the unstable, saddle-kind, middle steady states (Elnashaie and Yates, 1973; Elnashaie and Elbially, 1980). It was found (Kasat et al., 2002; Kasat and Gupta, 2003) that the sequential quadratic programming (SQP) technique using the ϵ -constraint method, failed to converge to the correct solutions, even though excellent starting guesses (near those provided by NSGA-II) were used.

Nandasana et al. (2003) optimized the industrial steam reformer reactor of Rajesh et al. (1999)] but under *dynamic* conditions, using NSGA-II. Two problems were studied to obtain the optimal operating conditions. A disturbance (in the form of a rectangular pulse) was introduced in the feed rate of natural gas (Problem 1) and in the inlet feed temperature (Problem 2). The decision variables used in Problem 1 were the furnace gas temperature, the steam-to-carbon ratio and the hydrogen-to-carbon ratio in the feed, while, in Problem 2, two additional decision variables were used: the time at the onset of the control action and the time at the cessation of the control action. Two objective functions were used in this work: the minimization of the *cumulative* deviations (over time) in the flow rates of (i) hydrogen and (ii) carbon monoxide (indirectly, of steam). An upper cap was imposed on the outer wall temperature of the reformer tube, as in the steady-state optimization study (Rajesh et al., 1999). A Pareto set of optimal solutions was obtained, once again. Again, this problem is extremely compute-intensive, and faster algorithms than NSGA-II are useful.

4.3 NSGA-II-JG

Kasat and Gupta (2003) recently introduced a modified mutation operator, borrowing from the concept of jumping genes (JG) in natural genetics. This algorithm is being called as NSGA-II-JG. This is a macro-macro mutation and counteracts the decrease in the diversity created by elitism.

Figure 3 (box indicated as JG) shows that the jumping genes operation is carried out after crossover and normal mutation in NSGA-II. A fraction, P_{jump} , of *chromosomes* (selected randomly) in the population, are modified by the jumping genes operator. A *part* of the binary strings in the selected chromosomes is replaced with a newly (randomly) generated binary string *of the same length*. The two ends of the set of binary digits to be replaced are generated using random numbers. The replacement (jumping) genes are generated using the same procedure as used for generating the members of the initial population. Only a single jumping gene was assumed to replace part of any selected chromosome. This, and the fact that the length of this jumping gene was identical to the original substring, are artifacts of the algorithm, and are different than the more general phenomenon in nature (which may be exploited in the future).

Kasat and Gupta (2003) used NSGA-II-JG to solve a two objective function optimization problem for the industrial FCC unit studied by them earlier (Kasat et al., 2002). The two objective functions used were (i) the maximization of the yield of gasoline and (ii) the minimization of the coke formed on the catalyst during the cracking of heavy compounds (to minimize catalyst decay and so, to reduce the production of CO). The decision variables were the same as used in their previous study. Fig. 3 shows the Pareto sets obtained using both NSGA-II and NSGA-II-JG. It can be noticed (Fig 3b) that the results at the 10th generation using NSGA-II-JG are as good as the results at the 50th generation using NSGA-II (Fig 3a). This helps save considerable amounts of the computation

time and is important for compute-intense multiobjective problems like that of the FCC units. In fact, these workers also found that NSGA-II-JG obtained the correct global-optimal Pareto set for a test problem having ten-decision variables (Zitzler et al. 2002) in which 21^9 local Pareto optimal sets exist (NSGA-II failed to obtain the globally-optimal Pareto solution). So the introduction of the improved JG operator not only improves the speed of convergence, but, at times, gives correct solutions which are missed by other algorithms. Recently, Lee et al. (2003) optimized an existing (and at the design stage) of an industrial ethylene reactor using NSGA-I, NSGA-II and NSGA-II-JG. They found that solutions for both NSGA-I and NSGA-II are scattered even after 200 generations. Moreover, solutions from NSGA-II have a tendency to move towards the ends of the Pareto while for solutions from NSGA-I tend to move towards center with the increase of generation. However, NSGA-II-JP resulted in more smoothed Pareto solutions evenly distributed. In addition, Pareto converged in 100 generations compared to 200 generations required for both NSGA-I and NSGA-II.

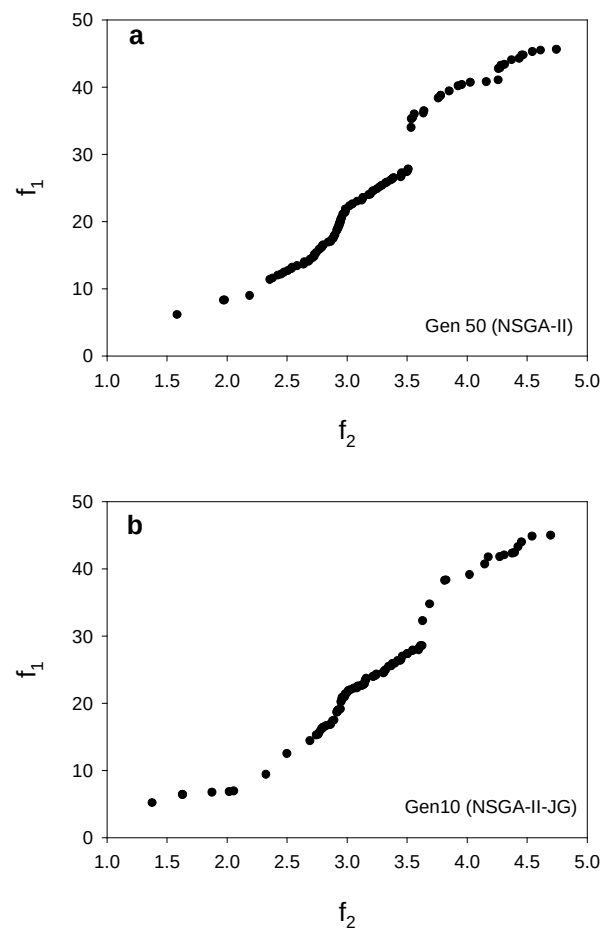


Figure 3. Comparison of the optimal solutions obtained for an FCCU by NSGA-II and NSGA-II-JG (Kasat and Gupta, 2003).

4.4 NON-DOMINATED SORTING SIMULATED ANNEALING (NSSA)

Simulated annealing (SA) is another emerging non-traditional algorithm (Kirpatrick et al., 1983; Aarts and Korst, 1989) which has been used for solving optimization problems in engineering. We expect SA to become quite 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 (a point). A neighbouring point is then created and compared with the current point. The probabilistic 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

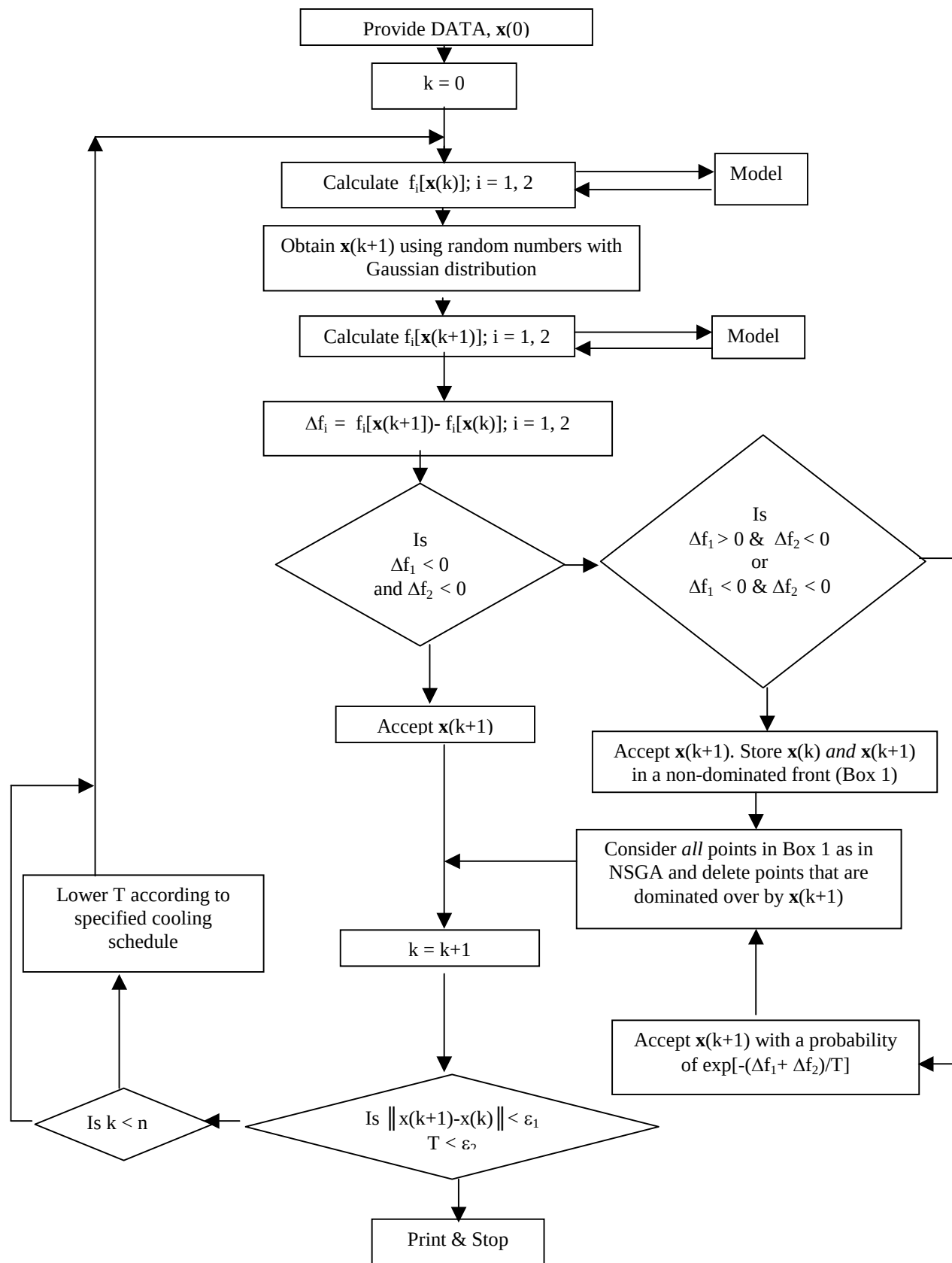


Figure 4. Flow chart for NSSA (Aatmeeyata and Gupta, 2003).

is created at each iteration exploiting the Boltzmann probability distribution. The method is found to be effective in finding unique, global optimal 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 of SA to compete with NSGA in terms of speed of convergence and robustness. The flow chart of the non-dominated sorting simulated annealing (NSSA, Aatmeeyata and Gupta, 2003) is given in Fig. 4, and is being tested for speed of convergence and spread of the Pareto points for some of the computationally intensive and industrially significant problems.

5. FUTURE DIRECTIONS

The three evolutionary algorithms, NSGA-I, NSGA-II and NSGA-II JG, are quite robust for generating non-inferior solutions for large-scale complex problems of industrial significance. 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- II 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

$[C_2]$	Cyclic dimer concentration in nylon 6 manufacture, mol/kg
DP	Degree of polymerization ($= \mu_n$)
$F_{CH_4, in}$	Flow rate of methane in the input stream of a steam reformer, 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
$F_{H_2, unit}$	Flow rate of H_2 in the exit stream from the reformer plant, kg/hr
$\mathbf{g}(\mathbf{x})$	Vector of inequality constraints, $g_i(\mathbf{x})$
$\mathbf{h}(\mathbf{x})$	Vector of equality constraints, $h_i(\mathbf{x})$
$\mathbf{I}$	Vector of objective functions, I_i
I_{dist}	Cowding distance
I_{rank}	Rank of any chromosome
L	Total length of the reactor
N_p	Number of chromosomes in the population in GA
p	Pressure
Q	Polydispersity index of polymer
t	Time
T	Temperature
V_T	Rate of release of vapor mixture from nylon 6 reactor through the control valve, mol/hr
$\mathbf{x}$	Vector of decision variables, x_i
x_m	Monomer conversion
z	Axial position in furnace reactor

SUBSCRIPTS / SUPERSSCRIPTS

av	Cross-sectional average value
d	Desired or design value
f, out	Final, outlet value
J	Jacket-fluid value
ref	Reference value
w	Wall or surface value

GREEK SYMBOLS

δ	fraction of steam used at the reactor inlet
λ	location of the injector port for the injection of steam
μ_n	Number average chain length of polymer

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