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<sup>\*,</sup> anjanadn@rediffmail.com

<sup>&</sup>lt;sup>†</sup>National University of Singapore, cheakr@nus.edu.sg

 $<sup>^{\</sup>ddagger}$ I I T Kanpur India, skgupta@iitk.ac.in

## 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 of tendepends 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 re 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 optimization of the reactor obviously needs to be minimized. However, additional important aspects need to be optimized simultaneously, e.g., process and products a fety, minimization of wastegeneration, 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 con ceptual levelarepresented 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) involv edtheeconomicefficiency, ascalar 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 sing le, 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 's calarization' 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. Whatiseven moreimportantisthatthereis ariskoflosingsomeoptimalsolutions(ChankongandHaimes, 1983; Haimes, 1977). The desirability function approach (Derringer, 1980; Deming, 1991) is another most widely used methods in industryfortheoptimizationofmultipleresponseprocesses.Iti sbasedontheideathatthe"quality"ofaproductor 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 firstintroducedtheconcept(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 oncopolymerization reactors (Butalaetal., 1988; Fanetal., 1984; Farber, 1986; Tso ukasetal., 1982).

## 3. PARETOSET

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

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$$\operatorname{Min} \mathbf{I}(\mathbf{x}) = \begin{bmatrix} \mathbf{I}_{1}(\mathbf{x}), \mathbf{I}_{2}(\mathbf{x}) \end{bmatrix} \tag{1a}$$

subjectto(s.t.):

$$\mathbf{g}_{\mathbf{j}}(\mathbf{x}) \leq 0, \mathbf{j} = 1, 2, \dots, \mathbf{J}; \tag{1c}$$

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

InEq.1, xrepresentsap -dimensional vector of pdesignor decision variables. It is found that the (feasible) solution of Eq. 1 often (but not always) comprises of several optimal solutions, 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,  $\mathbf{x} (\equiv [x_1, x_2, ..., x_p]), \text{ of }$ Eq. 1. The curve in Figure 1 is referred to as a Pareto set (Chankong and Haim es, 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). M ore 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. P oints A and C are no n-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, formethods to study these).

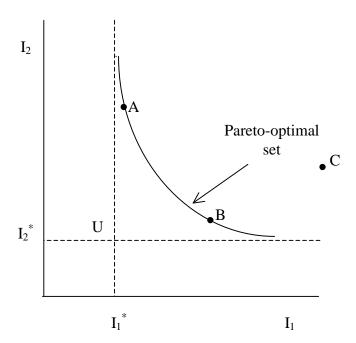


Figure 1. Diagram of Pareto optimal set for a two objective function optimization problem.

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  $_{i}$ \*=constant, can be obtained by solving the single objective function optimization problem in which wem in imize only I  $_{i}$ (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 whil ethe 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

needstominimizeanyobje ctivefunction, I i, one replaces it by the maximization of a fitness function, F i. Apopular transformation is  $F_i \equiv 1/(1+I_i)$ .

The second, subjective phase involves the selection of the preferred solution from a mong 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 (Nishi tani 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 tradeoffs between the nonce of the objective functions is equivalent to the degradation that results in the other objectives.

## 4.ALGORITHMSFORMULTIOBJECTIVEOPTIMIZATION

Extensiveresearchhas been reported on the algorithms used for generating the non--inferiorParetosolutions. 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; Hw ang 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 -basedGA(Haielaet 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 (Kitaetal., 1996), random -weightedGA(Murata, 1997), strengthParetoevolutionary algorithm (SPEA; Zitzler and Thiele, 1998), multiobjective messy GA (van Veldh uizen, 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 a dvantages 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 -IIandNSGA -II-JG, sincethese have been used exten sively inchemical reaction engineering.

## 4.1NSGA -IANDITSAPPLICATIONS

NSGA-I(SrinivasandDeb, 1995). This algorithm build supon the basic framework Inthissection, we first describe provided by Holland (1975). In NSGA -I, an initial population of s everal *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 do ne 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 -setof 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 **x**-spaceorinthe **F**-space.Anichecount(= informationonthedistancebetweenpair sofchromosomes, eitherinthe 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. Alter natively, we could use a suitable decreasing function (sharing function) of the distance from a reference chromosometoe valuate this niche count of "nearest" neighbours. In this latter approach, a neighbour that is farther contributes less to the niche co untthanone 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 valueassignedto allmembersofFrontNo.2should,obviously,besmaller(arbitrarilyagain)thanthelowestshared fitness value in Front No. 1. This procedure is continued till all the chromosomes in the population have been

assignedsharedfitness values. The use of the isprocedure 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., rou lette 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, a fter 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 spread of points. The flow chart of NSGA-I is available in Mitra et al. (1995). User -friendly codes of NSGA -I are available at <a href="http://www.iitk.ac.in/kangal">http://www.iitk.ac.in/kangal</a>.

NSGA-I has been applied extensively in chemical engineering. These have been reviewed r ecently 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 - Inchemical 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 usedweretominimize(i)thetotalreactiont ime,t f(subscript,f,indicatesfinal),and(ii)theconcentration,[C  $_{2}$ <sub>f</sub>, 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 aver age chain length,  $\mu_{n,f}$ , of the product so as to  $x_{m,d}$  and  $\mu_{n,d}$ , respectively. The decision variables used in this study were (i) obtainproducthavingthedesignvalues, therateofrelease, V <sub>T</sub>(t), of the vapor from the semi -batchreactor (a function of tim e,t) that influences the pressure history, p(t), in the reactor, and (ii) the jacket fluid temperature, T <sub>I</sub>(ascalar). The continuous function, V  $_{\rm T}(t)$ , was descritized into several, equi -spaced (in time) scalar values, V  $T_{i}$ ; i = 1, 2, ..., Q, and the value of V<sub>Ti</sub> was constrainedtolie(randomly)withinasmallrangeofthe previous value, V <sub>T,i-1</sub>, i.e., the permissible range of V <sub>T,1</sub> was much larger than those of the subsequent V T<sub>i</sub>. This enabled V <sub>T</sub>(t) to be implementable. Pareto -optimal solutions were obtained. Mitraetal. found that the solutions obtained by NSGA -Iwere superior to the se of Sareen and Gupta (1995), who had introduced artificial constraints by parameterizing the decision variables. They used Pontryagin's minimum principle. Interestingly, c onsiderable improvement in the operation of the reactor has been achieved industrially.

GuptaandGupta(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 Mitraetal. because the operat ion 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 (Aatmeey at a and Gupta, 1998).

Garg and Gupta (1999) applied NSGA -Ito the multiobje ctive 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 p olydispersity 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 importan ce since a controversy had existed on this point for several years, based on earlier optimization studies that used as calarobjective 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 conversionattheendofthefurnace,x <sub>m.av.f</sub>, 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, anypointinthe film must be below a  $\mu_{n \text{ av f}}$ , should be equal to ad esired value,  $\mu_{n,d}$ . In addition, the temperature at safe upper value, to prevent degradation (discoloration) of the polymer film. The decision variables used were the temperature of the isothermal PFTR, concentration o ftheinitiatorinthefeed to the PFTR, monomer conversion at the end of the PFTR, film thickness (all scalars), and the temperature programming, T  $_{\rm w}$ (z), in the furnace (a continuous *function*). In order to simplify the problem, the temperature of the surf ace of the film,  $T_{w}(z)$ , was parameterizedusingcubicfunctionsofz.

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 f unctions used were to minimize the concentrations of two undesirables ideproducts in the polymer, namely, the aciden dgroup and the vinylend 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 ob tained. 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.

Rajeshetal.(1999)carriedoutthemultiobjectiveoptimizationofanindustrialside -firedsteamreformerreactor (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 CH4.in, required 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 prob lem 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 t he gas mixture at the reformerinlet, pressure at the inlet of the reformer, steam to carbon (in the form of CH 4)ratiointhefeed,hydrogen (recycled H<sub>2</sub>) to carbon (as CH<sub>4</sub>) 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 specific bounds of the decision variables, these being decided based on experience with simulation runs. Rajeshet al.(2001)subsequentlyextendedthis work on the first reactor to the entire hydrogen plant (steam reformer reactor + two shift converters, etc.). Simultaneous maximizatio n 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. Ohetal. (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-gastotheunit, 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 (Ohetal., 2001) and design stage (Ohetal., 2002b) optimization. These workers found that the optimal solutions led to an improvement of the current operation of the industrial unit.

Yeeetal.(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

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. Paretooptimal solut ions 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  $_2$  (intermediate) products overcomplete conversion to C and CO  $_2$  products. Recently, Yuetal. (2003) optimized modified SCMCR systems, namely Varicol process (which is based on nonsynchronous switching) for synthesis of methylacetate ester. They reported much improved optimal solution overtraditional SCMCR .

## 4.2NSGA -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 apriori. The total complexity of NSGA -I is MN  $_{\rm p}$ <sup>3</sup>, where M is the number of objective functions, and N  $_{\rm p}$  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 rec ently 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 dominationusingadifferent procedure. Anewbox, P'iscreated, having size, N <sub>p</sub>. Achromosome (starting from the first)inboxPisremovedandcompared with all the solutions already presentinboxP'. AnychromosomeisP'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 kep tin P'. This is repeated with all N<sub>p</sub> 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 subset of those originally in P) is present in P'. This subset constitutes the first front or subset of those originally in P) is present in P'. This subset constitutes the first front or subset of the present in P'. This subset constitutes the first front or subset of the present in P'. This subset constitutes the first front or subset of the present in P'. This subset constitutes the first front or subset of the present in P'. This subset constitutes the first front or subset of the present in P'. This subset constitutes the first front or subset of the present in P'. This subset constitutes the first front or subset of the present in P'. This subs-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 -boxesof P' using the chromosomes remaining in P. Rank numbers, 2, 3, ..., are assigned to these fronts. In the present procedure, a comparison of the chromos omes is carried out *only* with the members present in the current sub -box. -assigning stepto  $MN_p^2$  operations. Thisreducesthenumericalcomplexityofthefront

The chromosomes in each of the fronts in P' are then arranged in ascending or derof 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 astogive them considerable weight).

 $Two chromosomes are now picked randomly from all the N \\ p chromosomes in P', and the better of these \\ two (having a smaller value of I \\ rank or, if I \\ rank are identical, having a larger value of I \\ p members. Clearly, m \\ ultiple copies (or no copy) of any chromosome in P' may be present in P''.$ 

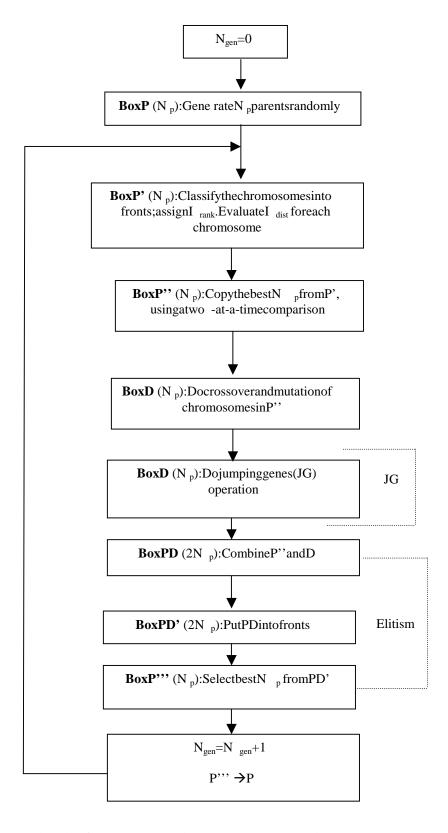


Figure 2. Flowchart for NSGA - II and NSGA - II-JG (Kasatand Gupta, 2003).

 $Chromosomes in P" are copied to a new box, D, having N \\ carried out on the chr omosomes in D. This gives N \\ _p daughter chromosomes.$ 

 $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 newbox, PD, having size 2N $_{p}$. These chromosomes are reclassified (and placed in PD') using $_{p}$ parents are selected and placed in box, P'''. This completes one generation and ensures the elite parents to be present. User NSGA-II are available at $_{p}$ 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 i ntensive problem, since it involves an iterative solution of the equations describing the two connected reactors: the riser -reactorandtheregenerator.NSGA -IIwasusedtosolvea three-objective function problem. The objective functions used were: maximi zation of the gasoline yield, minimization of the airflowrate to the regenerator, and minimization of the per -centCOinthefluegascomingout of the regenerator. A fixed feed (gasoil) flow rate was used. The decision variables used were: pre -heattem perature -heat temperature, circulation rate of the catalyst, and the flow rate of air. of the feed to the riser reactor, air pre Pareto optimal solutions were obtained. These correspond to the unstable, saddle -kind, middle steady states (Elnashaieand Yate s, 1973; Elnashaieand Elbialy, 1980). Itwasfound (Kasatetal., 2002; Kasatand Gupta, 2003) that the sequential quadratic programming (SQP) technique using the ε-constraint method, failed to converge to the correctsolutions, eventhough excellentstar tingguesses (nearthose provided by NSGA -II)wereused.

Nandasanaetal. (2003) optimized the industrial steam reformer reactor of Rajeshetal. (1999)] but under dynamic conditions, using NSGA -II. Two problems were studied to obtain the optimal operat ing 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 (Rajeshetal., 1999). A Paretoset of optimal solutions was obtained, once again. Again, this problem is extremely compute -intensive, and faster algorithms than NSGA -II are useful.

## 4.3NSGA -II-JG

Kasatand Gupta (2003) recently i ntroduced 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.

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

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

timeandisimportantforcompute -intensemultiobjective problems like that of the FC Cunits.Infact,theseworkers also found that NSGA -II-JG obtained the correct global -optimal Pareto set for a test problem having ten -decision 9 local Pareto optimal sets exist (NSGA) variables (Zitzler et al. 2002) in which 21 -II failed to obtain the glob 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 a t 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 endsoftheParetowhileforsolutionsfrom 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 generationsrequiredforbothNSGA -IandNSGA -II.

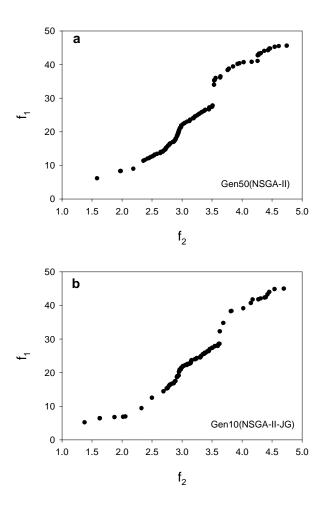


Figure 3. Comparison of the optimal solutions obtained for an FCCU by NSGA - II-JG (Kasatand Gupta, 2003).

## 4.4 NON-DOMINATEDSORTIN GSIMULATEDANNEALIN G(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 cur—rent 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 an expoint

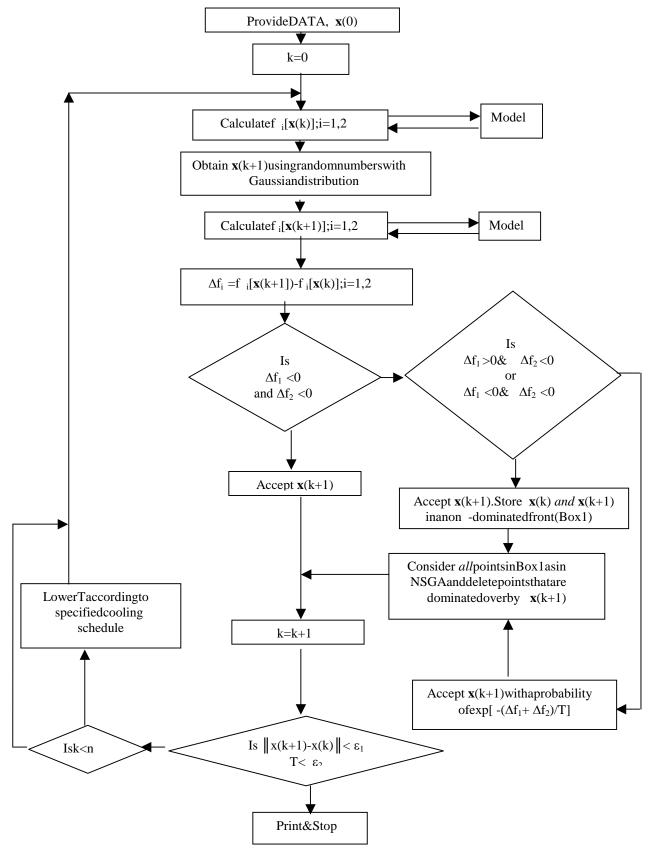


Figure 4. Flow chart for NSSA (A at meey at a and Gupta, 2003).

iscreated 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, so mew hat 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 an dindustrially significant problems.

### 5.FUTUREDIRECTIONS

The three evolutionary algorithms, NSGA -I, NSGA -II and NSGA -IIJG, are quiter obust for generating non 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 Pa reto 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**

$[C_2]$	Cyclicdimerconcentrationing	nylon6manufacture,mol/kg
DD	D C 1 ' ' /	

DP Degreeofpolymerization(=  $\mu_n$ )

F<sub>CH4.in</sub> Flowrateofmethaneintheinputstreamofasteamreformer,kg/hr

 $F_{CO,out}$  FlowrateofCOintheexitstreamofthefirstreact orinthereformerplant(inthesyngas),kg/hr

F<sub>H2,unit</sub> FlowrateofH <sub>2</sub>intheexitstreamfromthereformerplant,kg/hr

 $\begin{array}{lll} \textbf{g}(\textbf{x}) & \text{Vectorofinequalityconstraints,g} & _{i}(\textbf{x}) \\ \textbf{h}(\textbf{x}) & \text{Vectorofequalityconstraints,h} & _{i}(\textbf{x}) \\ \textbf{I} & \text{Vectorofobjective functions,I} & _{i} \end{array}$ 

 $\begin{array}{ll} I_{dist} & Cowding distance \\ I_{rank} & Rank of any chromosome \\ L & Total length of the reactor \end{array}$ 

N<sub>p</sub> Number of chromosomes in the population in GA

p Pressure

Q Polydispersityindexofpolymer

t Time

T Temperature

 $V_{T} \hspace{1cm} \textbf{Rateofreleaseofvapormixture from nylon6 reactor throught} \hspace{1cm} \textbf{he control valve, mol/hr}$ 

x Vectorofdecisionvariables,x i

 $x_m$  Monomerconversion

z Axialpositioninfurnacereactor

## SUBSCRIPTS/SUPERSC RIPTS

av Cross-sectionalaveragevalue
d Desiredordesignvalue
f,out Final,outletvalue
J Jacket-fluidvalue
ref Referencevalue
w Wallorsurfacevalue

#### **GREEKSYMBOLS**

- δ fractionofsteamusedatthereactorinlet
- λ locationoftheinjectorportfortheinjectionofsteam
- $\mu_n$  Numberaverage chain length of polymer

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