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Application of multi-objective optimization in the design and operation of industrial catalytic reactors and processes

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1 Introduction

Optimization in engineering is the search for the "best" solution to a specific problem. Criteria to determine whether the solution is the "best" or not vary widely and are defined by an engineer (researcher) based on their experience, the problem's objectives, common sense, etc. For example, while optimizing the performance of a synthesis reactor, it's often desired to maximize the possible yield of the final product; or in the case of equipment design, it is common to reduce the total cost while keeping a unit's performance at the desired level.

Engineering optimization can be classified by the number of objectives: either single-objective optimization (SOO) or multi-objective optimization (MOO). The SOO approach has a longer history. Essentially, it is based on the formulation of a unified function that represents the overall effect. Most of the objective functions in SOO are related to the economic efficiency of the process or unit. A classical example is the optimization of insulation thickness. Insulation saves money through reduced heat loss, but insulation can be very costly at the same time. One has to compare the total cost of new insulation with the savings from energy losses to find an optimal thickness; the ratio between these two factors can be an objective function to be minimized (Figure 1) [1]. It can be said that SOO methods are mainly aimed at a search for an extreme point (minimum or maximum) in a search space.

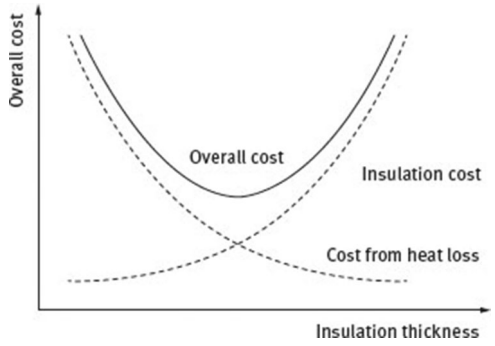

Figure 1: Overall economic effect of heat insulation.

However, it is not always possible to formulate a single objective for a particular problem that can adequately represent a meaningful and optimal solution. MOO methods appeared in order to overcome this drawback. One can deal with more than one objective, and these objectives are not necessarily economic-related parameters. For example, consider a very common reaction engineering problem in chemical engineering – simultaneous yield maximization of a goal (desired) product and the minimization of an undesirable side product. Such cases are quite common for oil refining, the petrochemical and polymer industry, organic synthesis, etc. Consider a simple parallel reaction, where we are targeting species B (desired) while species C is a side product (undesired):

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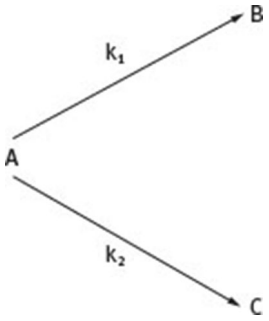

Operating conditions might have a similar effect on the yield of both products, e.g. an increase in process temperature, an increase in the percentage of both desired and side products in the outflow. Plotting this trend (concentration vs. temperature) (see Figure 2), it is possible to visualize the conflictive nature of our objectives: one cannot increase the concentration of B (desired) and decrease concentration of C (undesired) simultaneously. If we apply a classical single-objective approach, we would probably formulate the objective function in some way relating to the price of production to the concentrations of species. But, this type of objective function (cost minimization or profit maximization) usually is time- and/or site-specific. The cost of raw material or revenue generated from selling a product is site-dependent (price varies from one region to another around the globe) and time dependent (price varies from year to year).

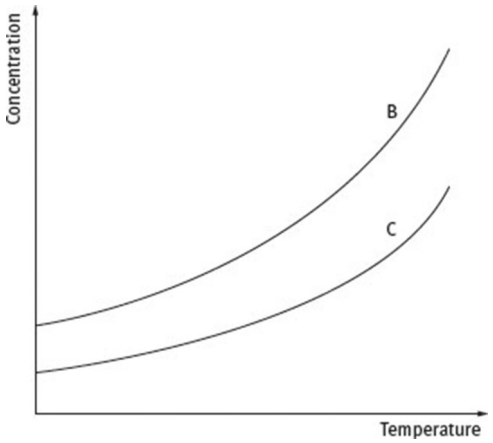

Figure 2: Effect of temperature on concentration of species in parallel reaction scheme.

Applying MOO methods allow one to solve such problem; one can directly treat product concentrations as objectives instead of a single objective function expressed in terms of economic effect (cost minimization or profit maximization). This is why a multi-objective approach is superior to a "classical" single objective approach.

In the current work, we will briefly consider the general ideas and concepts in use for MOO, the methods applied – especially more recent and state-of art ones – and complete a review of its applications in chemical reactor engineering.

2 Multi-objective optimization

2.1 Concept of multi-objective optimization

The multi-objective optimization (MOO) concept originates from economics and was developed by the Italian economist, engineer and philosopher Vilfredo Pareto. First let us consider the definition of multi-objective optimization of a minimization problem (here and throughout the chapter we will discuss minimization MOO problems, since any maximization problem can be converted into a minimization one quite easily):

$$\underset{x \in S}{\text{minimize}}\, I(x) = [I_1(x), I_2(x), \ldots, I_n(x)], \tag{1}$$

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subject to:

$$g_k(x) \leq 0, \quad i = 1, 2, \ldots, K,$$
$$h_j(x) = 0, \quad j = 1, 2, \ldots, J,$$

where n is the number of objectives, K and J are the number of inequality and equality constraints respectively, **x** is a vector of decision variables in a search space **S**. A general solution for such an optimization problem is a set of points instead of a single one such as in SOO problems. However, in some special cases, a single point solution is also possible, which we will not consider for this trivial case. The set of points is called a Pareto set (front or distribution).

Definition of a Pareto optimal point

A point **x** is called a Pareto optimal point if and only if such a point **x*** doesn't exist in a search space in which I_i (**x***) is "better" than I_i (**x**) for all objectives simultaneously. By "better" it is necessary to assume mathematical operators $\leq$ or $\geq$ depending on the particular problem formulation.

A Pareto set can be presented in terms of decision variables (set of **x**) or objectives (set of I(**x**)). For a better understanding, let's illustrate a Pareto concept for a two objective function problem (Figure 3). If the problem requires simultaneous maximization of both objectives A and B, Figure 3 describes the Pareto set obtained with respect to decision-variable limits and equality and inequality constraints. If we move from point 1 to point 2, objective A is increasing (desired) while objective B is decreasing (undesired). It is said that these two points like any other points on the curve are non-inferior (non-superior or equally good) to each other. If we move from point 3 in the direction of Pareto, one can see that both objectives A and B are improving, thus point 3 is not a Pareto point.

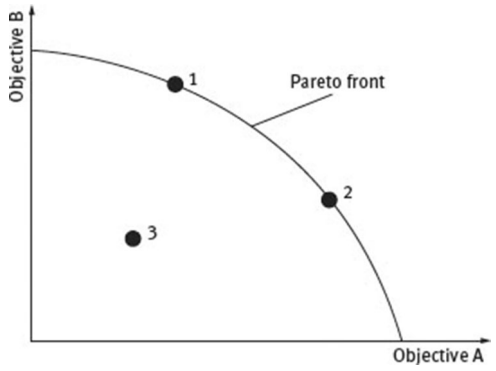

Figure 3: Pareto set for two conflicting objectives.

2.2 MOO methods

When we have determined a solution for a MOO problem in the form of a Pareto set, let us turn our attention to methods utilized for its search. There are a number of different techniques; later, we will provide the accepted classification of them for better understanding [2–4]. The classification is based on a decision maker's (DM) role in the optimization search. Here the DM is a person familiar with the formulated problem; he/she can impact on the preference of objectives or solutions. Therefore, methods are divided into:

– no-preference;

– *a priori;*

– *a posteriori;*

– interactive.

The first group excludes any influence of the DM on a search of Pareto points while the next two take it into account. The latter case is a group of currently developing methods in which DM is directly involved in the optimization search and is able to alter the preferences until the best solution is found. Just note here as a remark that the classification is not strict because the same methods can be referred to by more than one group; this will be shown later. From here we provide further a concise review of introduced methods.

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3 No-preference methods

If preferences are hard or impossible to define by DM, no-preference methods can be applied. They allow for finding "average" solutions regardless of any preference; no extra knowledge has to be provided by DM to solve such a MOO problem.

3.1 Neutral compromised solution

The neutral compromised solution method allows for finding optimal solutions "somewhere in the middle" of a Pareto set. To apply this technique, it is required to define the norm in an objective domain, which will be a measure of distance for the "middle" solution and the selection of a reference point from which the distance shall be minimized [5]. However, we can say that the DM expresses preferences by choosing the norm and reference point, but he/she is not doing it in an explicit way. For MOO problems, it is necessary for all objectives to be of the same dimension or dimensionless. The commonly used norms are p-norm, Chebyshev norm or an augmented Chebyshev norm. The following problems are to be minimized respectively:

$$\begin{aligned}
&\underset{x\in S}{\text{minimize}} \left[\sum_{i=1}^{n} \frac{\left|I_{i,\text{up}} - I_i\right|^p}{\left|I_{i,\text{ up}} - I_{i,\text{ low}}\right|^p}\right]^{1/p}, \quad 1 \le p \le \infty, \\
&\underset{x\in S}{\text{minimize}} \max_{1\le i\le n} \frac{\left|I_{i,\text{ up}} - I_i\right|}{\left|I_{i,\text{up}} - I_{i,\text{low}}\right|}, \\
&\underset{x\in S}{\text{minimize}} \max_{1\le i\le n} \frac{\left|I_{i,\text{ up}} - I_i\right|}{\left|I_{i,\text{ up}} - I_{i,\text{low}}\right|} + \varepsilon \sum_{i=1}^{n} \frac{\left|I_{i,\text{up}} - I_i\right|}{\left|I_{i,\ up} - I_{i,\text{ low}}\right|},
\end{aligned} \tag{2}$$

where ε is a small number > 0. The denominator in each term plays the role of a scaling factor for minimizing the distance between upper $I_{i,\text{up}}$ and lower $I_{i,\text{lower}}$ values for each objective function. Also, a *method of global criterion* is one of such methods but will be considered in section on *a priori* methods below with some remarks.

4 *A priori* methods

A priori methods require the DM to state his preference in a MOO problem. This has to be done prior to determining the Pareto set. One can specify the priority of objectives (or aims) to be achieved. Since a DM is a person familiar with a particular problem, sometimes it becomes possible to single out more important objectives or put them in an order of preference.

4.1 Method of Weighted global criterion

This method with some variations is the most popular technique for a MOO. The idea is to transform objective functions into a single one, thereby scalarizing the search space. In the most general form, this method can be written as

$$\underset{x\in S}{\text{minimize}} \sum_{j=1}^{n} F\left(I_j\left(x\right), w_j\right). \tag{3}$$

A scalarized function represents the sum of composite functions of objective I_i (**x**) and weighting factor w_i. The latter itself is a measure of the DM's preferences for a particular objective. Usually weighting factors are assigned in such a way that $\sum_{j=1}^{n} w_j = 1$ and $w_j > 0$. In a simplest form, the expression (1) can be written as a weighted exponential sum [4]:

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$$\begin{aligned} &\underset{x\in S}{\text{minimize}} \sum_{j=1}^{n} w_j \left[I_j(x)\right]^p, \ I_j(x) > 0, \\ &\underset{x\in S}{\text{minimize}} \sum_{j=1}^{n} \left[w_j I_j(x)\right]^p, \ I_j(x) > 0. \end{aligned} \tag{4}$$

Note that in the case of Eq. (3) with $p = 1$ (because of its simplicity), it is called the method of a weighted sum and widely used in applied chemical engineering problems [6].

Some other modifications are required for the idea of a utopia point, $I^{\text{utopia}}(\mathbf{x})$; the imaginary point in a search space where all the objectives reach a minimum value simultaneously. The aim is to minimize the weighted distance between the objectives and that point [7]. Different metrics can be used as a distance measure. Often this group of techniques is called weighted metrics [3]. Here we provide some of them:

$$\begin{aligned} &\underset{x\in S}{\text{minimize}} \left[\sum_{j=1}^{n} w_j \left(I_j(x) - I_j^{\text{utopia}}(x)\right)^p\right]^{1/p}, \\ &\underset{x\in S}{\text{minimize}} \left[\sum_{j=1}^{n} w_j^p \left(I_j(x) - I_j^{\text{utopia}}(x)\right)^p\right]^{1/p}. \end{aligned} \tag{5}$$

Note here that instead of a utopia point, the DM can determine a set of objectives that one desires to reach. This makes sense from a practical point of view, or when the real utopia point is unknown.

Remarks: A group of weighted global criterion methods is also a popular *a posteriori* technique. By varying the weights, it is possible to obtain a Pareto set instead of a single point. These methods always converge to a Pareto optimal solution, but an entire Pareto set can not be found if the problem is not convex [3]. If one assigns all weights, w_i, equal to 1, the approach can be classified as no-preference; but the drawback remains the same. In addition, the magnitudes of objective values should be commensurable with each other to avoid overemphasis of one over the other. Hence, normalization is required for applying this technique [3].

4.2 Lexicographic method

Lexicographic methods require the DM to sequentially organize objectives from 1 to N in terms of preferences [8]. The following problem has to be solved [4]:

$$\underset{x\in S}{\text{minimize}} \, I_i(x), \tag{6}$$

subject to:

$$I_k(x) < I_k\left(x_k^*\right) \ k = 1, 2, \ldots, i-1; i = 1, 2, \ldots, n,$$

where k is the function order in a preference list, $I_k\left(x_k^*\right)$ the constraint's limit received at k^{th} step. The first objective in the list should be minimized with the original constraints. If the DM obtains a single solution, one can accept it as an optimum. If not, the new constraint $I_k\left(x_k^*\right)$ has to be accepted to keep the k^{th} objective's optimal values. The procedure continues with the next objective function (e.g. second function in a list, third function in a list, etc.), until the optimum is reached.

In reality, it is often difficult for a DM to distinctly organize objectives in an order of importance on account of the complexity of a MOO problem. Another drawback with this technique is that a unique solution is often found before the best optimal solution is reached. It means that some of the objectives are not taken into consideration at all [3].

4.3 Goal Programming (GP)

This method was developed by Charnes and Cooper [9]. The DM defines a set of goals **G** that should be achieved for each objective I_i (**x**). Even if all these goals are unattainable simultaneously, it is still desired to reach them

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"as close as possible". It is proposed to minimize the distance between vectors **I**(**x**) and **G**. Such a weighted GP problem formulation is written as:

$$\begin{aligned} &\underset{x\in S}{\text{minimize}} \sum_{i=1}^{n} w_i \delta_i, \\ &\delta_i = I_i(x) - g_i, \quad i = 1, 2, \ldots, n, \end{aligned} \tag{7}$$

where w_i is a weighting factor for objective I, is a deviation of objective I_i (**x**) from goal g_i. The formulation of this goal programming problem doesn't necessarily require the solution to be Pareto optimal. The solution obtained can be referred to as: (a) efficient; (b) inefficient; or (c) an unbounded solution. An efficient solution belongs to a Pareto front while an inefficient solution can be improved for two or more objectives simultaneously. The latter case is a solution located too far from a Pareto front [10].

Setting goals is a clear approach for a DM (unlike, for example, the use of a utopia point in the global criterion method). However, the further procedure for an optimum search is not necessarily easy, e.g. weights assignment can be more difficult. Some GP methods are combined with a lexicographic method, where deviations are structured in preference order and then minimized. The DM has to be aware of all the drawbacks of GP methods and choose the proper technique for finding an optimal solution.

5 *A posteriori* methods

In contrast to other methods discussed so far, an *a posteriori* method generates a Pareto set first, when the DM is given the opportunity to choose acceptable ones. It is reasonable if the DM is unsure about his/her preferences, or the problem definition is vague about the relative importance of objectives.

5.1 ε-Constraint Method

The ε-constraint method is a non-scalarizing approach. The original idea was reported by Yacov Haimes [11]. The more comprehensive explanation is provided by Chankong and Haimes [12]. It is proposed to solve the following n-objective problem (Eq. (1)) to define a Pareto set:

$$\underset{x\in S}{\text{minimize}}\, I_i(x), \tag{8}$$

subject to:

$$\begin{aligned} I_m(x) &\le \varepsilon_m, \quad i = \{1, 2, \ldots, n \setminus m \neq i\}, \\ g_k(x) &\le 0, \qquad i = 1, 2, \ldots, K, \\ h_j(x) &= 0, \qquad j = 1, 2, \ldots, J, \end{aligned}$$

where ε_m are user defined constraints. Note that any of the objective functions can be chosen for minimization. By varying ε_m, the Pareto set can be reached. It is reported by authors that the current method can deal with non-convex problems. However, drawbacks still exist. The choice of ε_m is not as easy for DM; the technique also significantly increases computation time if the total number of equations (objectives and constraints) is relatively high.

6 Interactive methods

As it follows from the name, interactive methods require some sort of interaction between the DM and the MOO algorithm. Initially, no *a priori* information is required, and the DM specifies some objective-related preference information during a search process. Solutions in interactive methods move iteratively, providing the DM with some new solution(s) and allowing the re-specification of his/her preferences, if needed. The interactive methods outcome is one or more Pareto optimal solutions, but not the entire Pareto set. Generally, many other variations exist, which are a kind of extension of classical methods described here with the way how DM should interact with an algorithm. There is a variety of such methods and we will not discuss it here providing only references on some original sources and reviews:

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– interactive Surrogate Worth Trade-off (ISWT) [12];
– reference point methods [13];
– non-differentiable Interactive Multi-objective Bundle-based Optimization System (NIMBUS) [14];
– step method (STEM) [15].

For an overview of interactive methods, we refer the reader to outstanding reviews by Miettenen [16] and Branke *et al*. [3].

7 Genetic algorithms

Genetic algorithms (GAs) are currently one of the most developing groups of methods in MOO. They are "based on the mechanics of natural selection and natural genetics" [17]. Here, we would like to emphasise the power of GAs and discuss them in more details. However, genetic algorithms belong to *a posteriori* methods; we discuss GAs in an individual sub-chapter on account of their fundamental difference to the methods discussed above.

The original idea was proposed by Holland [18] as an adaptation concept. Thereafter, Goldberg evolved this theory and formulated general regulations of GAs [17]. GAs have been developed intensively in recent years, but the main principles remain the same. As indicated by Goldberg, main distinctions from classical methods are:

– GAs work with a number of points (population) instead of a single one;
– GAs treat objective functions directly; there is no need for derivatives, utility functions, or any other auxiliary knowledge;
– GAs operators are probabilistic in nature in contrast to deterministic ones used in all classical methods.

GAs are notable for their robustness. It is a superior search procedure in many aspects. Unlike many derivative-based methods that can be trapped around local optima, GAs are a global optimum search procedure. They can also treat discontinuous or discrete functions. they overcome issues with the convexity of a Pareto set as well as deal with multi-modal objective functions [19].

7.1 About binary-coded variables

Preceding the explanation of GAs' working principles, one has to know about binary-coded variables. The most common representation of a variable utilized by GAs is a binary string. That variable is simply a certain length sequence of ones and zeros (e.g. 1001). If a user deals with continuous variable (e.g. length, product yield, time, etc.), it is required to discretize the variable. The procedure is quite simple. For example, the decision variable $x \in [X_{\min}, X_{\max}]$ has to be mapped into a binary string. The user decides to use 4 bits for each variable, in other words, the length of binary string is set to 4 digits. Thereby, we have $2^4 = 16$ possible combinations of strings. Lower and upper bounds are assigned with the values $X_{\min} \rightarrow 0000$ and $X_{\max} \rightarrow 1111$. All other values are mapped in between these two values (Figure 4).

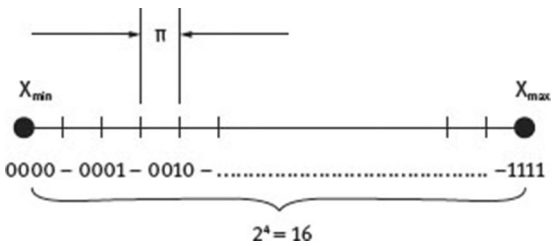

Figure 4: Mapping of real value into binary variable.

The precision of discretization of variables is directly dependent on the string length; the longer the length, the more binary variables can be mapped between the lower and upper limit. The precision π may be calculated as [17]:

$$\pi = \frac{x_{\max} - x_{\min}}{2^{l_{\text{str}}} - 1}. \tag{9}$$

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7.2 Simple Genetic Algorithm (SGA)

For a better understanding the GAs' principle, let us consider a simple genetic algorithm (SGA) first. The main components of a SGA include: (a) reproduction; (b) crossover; and (c) mutation of genetic operators. At the beginning, the initial population is generated randomly. The population is a set of individuals; each of which represents a single decision variable (or a vector). The reproduction operator is applied to the population to create a "mating pool". Individuals with a higher objective function value have a higher chance of being copied into a matting pool. Classical and simple way to perform a reproduction operator is a roulette wheel [17].

Once the mating pool is formed, crossover and mutation operations are executed. In a single point crossover, two individuals (called parent chromosomes) are chosen randomly to exchange "information" with each other. They swap binary sequences after the arbitrary position p (which is randomly selected) and then generate "daughter chromosomes" (Figure 5).

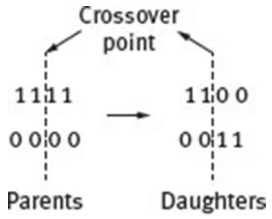

Figure 5: Representation of single point crossover between two binary strings.

Mutation is also aimed at altering the daughter chromosomes' binaries but in a different manner. Like mutation in nature, it occurs with a very small probability. Mathematically, it alters one cell in a sequence each time from 0 to 1 or vice versa. It is absolutely necessary to keep diversity in the population [20]. For example, let's assume a case where all individuals in a population have 0 at k^{th} position, under these conditions the crossover operator cannot create 1 at this point. Mutation allows one to overcome this issue.

The best n daughter individuals are taken to form a new mating pool where crossover and mutation are carried out again. This procedure repeats until the termination criterion is satisfied. Below we provide a generalized scheme of SGA (Figure 6).

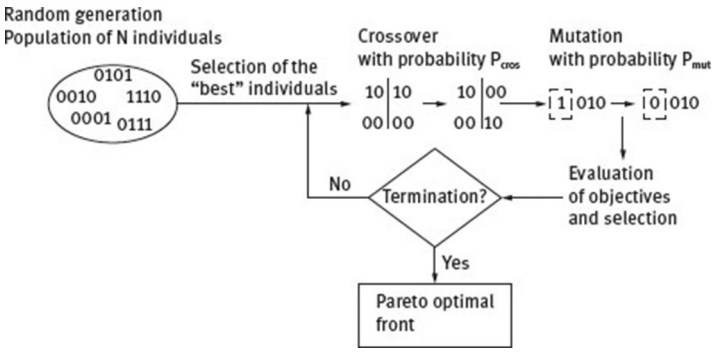

Figure 6: Simple genetic algorithm.

7.3 Use of GA in MOO

If one has a SOO problem, it is easy to choose the best solutions from the population by comparing the single objective values of individuals. When one deals with multiple objectives, it is not clear how to compare them. To deal with this, Goldberg introduces the concept of non-dominated vectors [17]. Vector **a** is said to be less than vector **b** if and only if these two conditions are satisfied simultaneously:

– all components of **a** are less or equal to corresponding components of **b**;

– at least one component of **a** is strictly less than corresponding element of **b**;

or, in other words (for a minimization MOO problem), **a** dominates **b**. If for the vector **a** there is no such vector **c** that dominates it, vector **a** is called non-dominated. From this point of view, a Pareto set is a non-dominated set.

Recent GAs' modifications are more complex than a SGA. There is diversity of different algorithms presented in the open literature: Vector Evaluated Genetic Algorithm (VEGA) [21], Multi-objective GAs (MOGA)

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[22], Strength Pareto Evolutionary Algorithm (SPEA) [23], Niched-Pareto GAs [24], Predator-Prey Evolution Strategy [25], Rudolph's Elitist Evolutionary Algorithm [26], NSGA-II [27], Differential Evolution (DE) [28] based methods and many others. We will not discuss most of them here, but refer readers to original sources.

We would like to emphasize one of the state-of-the-art algorithms: the non-dominated sorting genetic algorithm II (NSGA-II). The reader can note that this algorithm was used in a majority of MOO problems solved in the literature (Table 1). After development by Deb [27], it has been widely propagated in optimization problems for chemical engineering as well as for many other fields. NSGA-II is notable for its characteristics, especially its ability to find diverse solutions close to a real Pareto set and the speed of convergence [27]. Here are the elements that contribute to its high performance.

- This algorithm uses the concept of elitism. After mating pool formation, N parents and N daughters' chromosomes are united into a single group of $2N$. Selection is carried out over this pool and not only from the original mating pool. If parents are better than their daughters, it allows them to not be excluded them from population, but carry on in the next generation. This allows diversity.
- The Non-dominated Sorting Approach is used as a selection procedure. It divides an entire population into groups of non-dominated individuals (*non-dominated fronts*). Any solution in front 1 is superior to any solution in front 2, and so on.
- To maintain the diversity of the population, authors introduced crowding distance. If some region in an objective domain is too populated with individuals, it is reasonable to exclude some of them from the population. The crowding distance of point i represents an average side length of n-dimensional cuboid in objective space, drawn out around point i where two neighboring points are taken as vertices. The higher the crowding distance, the less crowded a region. Points from the same front but with less values than this parameter have less chance to carry on into the next generation. A step-by-step guide to execute NSGA-II, a performance of the algorithm in test problems or other characteristics can be found elsewhere [19, 27].

7.4 Constraint handling in GA

There are different techniques aimed at constraint handling in GAs. Constraints impose extra conditions on a MOO problem, thereby limiting the search space. Based on this, solutions are divided into feasible and infeasible regions. An infeasible solution cannot be neglected in GAs in order to maintain diversity. Even if a particular solution violates constraints, it should have a chance to remain in the population in order to have a chance to move to a feasible region [19]. To do this, many techniques evaluate the extent of violation from a feasible region. Two noteworthy techniques are discussed below, which have been utilized more frequently while solving applied MOO problems in chemical engineering.

Penalty function approach

The penalty function approach modifies the original objective functions by adding a constraint violation to them as follows [20]:

$$\underset{x\in S}{\text{minimize}}\, P(x) = I_i(x) + \Omega(R, g(x), h(x)), \tag{10}$$

where $I_i(\mathbf{x})$ is the original objective function, Ω is a penalty term, R is a penalty parameter. The penalty term represents the sum of constraint violations $v_i(\mathbf{x})$ from a feasible region:

$$\Omega = R\sum v_i(x).$$

Constraint violations $v_i(\mathbf{x})$ could be defined as:

$$v_i(x) = \begin{cases} |g_k(x)|, & \text{if } g_k(x), \\ 0, & \text{otherwise,} \end{cases} \tag{11}$$

or

$$v_i(x) = |h_i(x)|^2. \tag{12}$$

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The penalty parameter R is used to have values $I_i(\mathbf{x})$ and Ω of a similar magnitude. Hence, if a particular solution overruns a feasible region, the value of the penalty function $P(\mathbf{x})$ increases even if the value of the original objective function $I_i(\mathbf{x})$ is small. The solution becomes inferior and has a higher chance of being excluded from the population. One of the main drawbacks of this method is that the penalty function distorts the Pareto front of the original function which cause difficulties finding a true Pareto set.

Constrained tournament method

The constrained tournament method is a methods developed for use with GAs only. The approach can treat constraints directly instead of using any objective function transformation. It modifies the tournament selection of individuals for the formation of a mating pool. Now solutions are checked for constraint violation in addition to dominance. Between two infeasible solutions, the one chosen is the one with less constraint violations. When two individuals are picked for a tournament selection, the following "*constraint-domination*" rules have to be kept:

- the feasible individual is always superior to the infeasible individual;
- between two infeasible individuals the one with smaller constraint violation should be given priority; and
- if both individuals are feasible, the regular (non-constraint) approach should be applied.

The generic "*constraint-domination*" principle can be used with any GAs and doesn't require extra computational time [19].

4.8 Simulated annealing

Simulated annealing (SA) is another stochastic-based method of search and, like GAs, belongs to *a posteriori* methods. The procedure mimics the behavior of molten metals cooling. At high temperatures, metals behave like a liquid where atoms are in chaotic motion. When the cooling is started, atoms lose mobility and begin to form crystalline lattice of solid metal. The rate of cooling strongly affects the structure of crystal, the slower the rate, the more uniformed the structure. Uniformed mono-crystalline structure is more stable (i.e. has minimum energy).

SA for optimization was considered in [29]. They applied principles of statistical mechanics of systems in thermal equilibrium to solve the optimization problem. The main principle is based on the Boltzmann probability distribution function. At a given temperature T, the probability of the system to have energy E_1 is proportional to $\exp\left(\frac{-E_1}{kT}\right)$, where k is the Boltzmann constant. In this context, probability for a system to move from *state 1* to *state 2* is given as:

$$\frac{\text{state 1}}{\text{state 2}} = \exp\left(\frac{-(E_2 - E_1)}{kT}\right). \tag{13}$$

Hence, if E_2 is lower than E_1, then the system definitely turns to state 2. At the same time, if $E_2 - E_1 > 0$ a finite probability for transition from 1 to 2 still exists. The higher temperatures T correspond to higher probabilities of state 2 to exist. For energies in Boltzmann distribution equations, the reader has to consider objective values.

SA in the simplest form can be described in the following way: the algorithm starts with an initial point x_0 (usually random). The random point x_1 is generated in the neighborhood of x_0 and the objective values are compared at these points. If a new point improves our objectives, it is accepted instead of x_0. If not, the point x_1 is accepted with the probability $\exp\left(\frac{-(E_2 - E_1)}{kT}\right)$. During the search, the temperature T is slowly decreased ("cooling") which reduces the probability of a new point with worse objective being accepted. The search continues until some termination criteria are reached, for example, it can be an error between points in subsequent iteration or minimal temperature. One run of SA yields one Pareto optimal solution. Thus multiple simulations are required to obtain a Pareto set.

The same principle with some modifications can be applied for MOO problems [30–33]. Algorithms could differ in probability functions or stopping criteria, or they have some operators for a better Pareto distribution. The current technique is less popular than GAs but still has a significant interest in modern MOO applications.

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4.9 MOO problems in chemical engineering

The popularity of GA methods experienced significant growth since the end of the 1990s when they began to be implemented. The majority of research in chemical engineering optimization used GAs as a main technique in search of Pareto optimal solutions, however some other techniques were also used. Some comprehensive reviews of early applications are provided at Bhaskar *et al*. and Nandasana *et al*. [6, 34]. Here we will focus on a review of MOO problems and their solutions made in a recent decade for chemical reactors and process engineering. Some more widely presented MOO problems in open literature will be described below. Other MOO problems with objectives, methods and general remarks will be summarized in an auxiliary table at the end of chapter. We recommend readers to refer to original sources if interested in order to have a detailed description of a particular problem. Here we just summarize the main applied issues and concepts of MOO in chemical engineering and of their solutions.

It can be seen that even though reactors have different designs and arrangements, the processes have different foundations – continuous or batch type, homogeneous or heterogeneous, in gas or liquid phases, etc. Despite this fact, there are some general concepts that are used for MOO. For example, the most desired intention is to increase the production of a main product (e.g. in terms of yield or selectivity) and minimize side product formation. This usually affects some quality parameters of the product, which becomes a conflicting objective. Additionally, it could be related to a change in heat duties of heat exchangers, the fuel rate into furnaces or other similar parameters. Different scenarios and conflicting objectives could make the formulation very complex. Researchers/engineers are free to choose which objectives have higher importance and have to be given more consideration from practical point of view. In some way, proper MOO formulation itself is an "art" and can play a key role in finding meaningful and appropriate solutions.

4.9.1 Petroleum Processing Engineering

Noticeable contribution to GA and its application to MOO in petroleum processing was made by Kasat *et al*. [35]. They introduced a genetic operator called a Jumping Gene (JG). A JG (or transposon) mimics the real nature phenomena discovered in 1987 by McClintock. The main point of the discovery was that transposon is a DNA sequence which can randomly migrate among chromosomes and replace existing sequences. One of the transposon roles is providing for diversity in genotype. The jumping gene was introduced as a binary sequence that can replace a part of the original individual. First, the chromosome is checked for carrying JG out with some probability P_{JG}. If the condition is satisfied, two positions of binaries, p and q, are randomly chosen in the current chromosome with a total length l_{str} ($p < q \leq l_{\mathrm{str}}$). The random binary string of length $(q - p - 1)$ is generated and inserted between p and q. Another alternative for JG is to inverse binary sequences between chosen locations. It is reported that these two modifications have the same performance. Authors suggested to implement a JG operator after mutation and combine this operator with NSGA-II (NSGA-II-JG). Using benchmark problems, they demonstrated that the proper choice of P_{JG} (≈ 0.5 or more) provides a faster convergence to a Pareto front and better distribution of the population along it. The JG concept was developed in some later works [36–38] where new modifications with improved characteristics were introduced. We will not describe all of them in detail; we refer readers to the original articles.

In their work, NSGA-II-JG was applied for multi-objective optimization of an industrial fluidized catalytic cracking unit (FCCU). The FCC is very relevant for the petroleum processing industry since it is the main process for gasoline production. Industrial FCCUs consist of a reactor-riser and catalyst regenerator. Authors used a five-lump kinetic scheme with two steady state models of these units, previously developed and verified by Arbel *et al*. [39] and Krishna and Parkin [40]. The two objectives were to maximize the yield of gasoline from the FCCU and minimize coke content on the catalyst. The decision variables used were feed temperature and the catalyst flow rate into the reactor, as well as air temperature and flow rate into the regenerator with lower and upper bounds based on process technology. Again, the problem was solved with both NSGA-II and NSGA-II-JG. The obtained results were compared with their previous work [41], where optimization was carried out with original NSGA-II. The generated Pareto fronts ware similar but with a wider distribution of solutions for NSGA-II-JG. Authors emphasized computational efficiency and the speed of convergence and proposed methods for MOO problems in chemical engineering.

Some other petroleum processing MOO are presented in the open literature. Various researchers investigate MOO problems for different types of naphtha catalytic reformers, such as conventional catalytic naphtha reactor (CR) or the thermally coupled fluidized bed naphtha reactor (TCFBNR) [42–45]. Besides the designation for feed conversion into products, the naphtha reforming process could be aimed at a refinery's hydrogen supply. Because of this, objectives can vary from one reformer to another, depending on their roles in particular productions. In the majority of research, it was proposed to maximize the production of aromatic compounds

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and hydrogen while other objectives differed. However, only Weifeng *et al*. [42] treated objectives directly with a Neighbourhood and Achieved Genetic Algorithm (NAGA) to generate an entire Pareto set. Other researchers used summation method to form the SO function, and solve it with methods of differential evolution. All of them could provide improved objectives and propose a better operation conditions for naphtha reformers than current ones.

4.9.2 Steam Reforming

The first multi-objective optimization of a side-fired steam reformer was performed by Rajesh *et al*. [46]. They combined the kinetic model of main reactions, a heat transfer model through a furnace tube wall and the diffusion model in a catalyst pellet. The complex model was utilized for optimization. Authors assumed that the rate of hydrogen production was kept at a required level. The main operational costs of steam reforming are: (a) methane feed; (b) furnace fuel; and (c) steam. The first objective used was the minimization of the methane feed rate. The second objective used was the maximization of CO in the reformer outflow. The reason for this was that the higher the CO % in outflow, the more heat can be generated at the shift converter and, consequently, more steam can be produced in heat exchangers at the exit of the unit. Decision variables used were the temperature and pressure of the feed flow and its rate, steam/methane ratio (S/C), recycled hydrogen/methane ratio (H/C) and temperature of the furnace gas. Additionally, the process was constrained by a maximum possible furnace wall temperature. Thus, they came up with two objective problem formulations subjected to lower and upper boundaries for decision variables based on process technology and one constraint. The objectives and constraints were treated in the form of a penalty function. A Pareto set was obtained. It was noticed that most of the decision variables didn't differ significantly for an entire Pareto, but that the S/C ratio makes a significant contribution to the objectives value and for the Pareto distribution. They also studied the effect of catalyst deactivation on the change in optimal parameters. This change wasn't important due to thermodynamically controlled reactions. Generally it was shown in the work how to apply MOO with GAs to optimize the steam reformer. More precise problem formulations (e.g. constraints, process parameters limits, etc.) for a particular steam reformer can bring different results.

The work of Nandasana *et al*. [47] extended the optimization of a steam reformer dynamic regime. The existing model was modified as a non-steady state to study the effect of disturbances on the reformer. The objectives of MOO were to minimize the reduction of loss of the total (a) hydrogen and (b) steam production caused by a sudden change in some process parameters. Two disturbances were independently introduced to the system: a step decrease of methane feed; and a drop in feed temperature. Authors reported the high computational intensity of MOO problems. They could carry out 9 and 18 generations for the problem respectively.

In more recent research, Ebrahimi *et al*. [48] performed MOO of a steam reforming arrangement for the synthesis gas production (mixture CO and H_2). They modeled two combinations of top-fired methane steam and auto-thermal reformers, parallel and in series. They formulated objectives similar to Rajesh *et al*. [46]: (a) maximize production of syngas; (b) minimize furnace fuel consumption; and (c) minimize CO_2 releases. Like in previous research, the main constraint for the steam reforming operation was the maximum tube wall temperature. Obtained Pareto sets showed that a parallel arrangement is superior for higher syngas production while the configuration in series allows for a decrease of fuel consumption and CO_2 release.

4.9.3 Polymer industry

MOO in polymer manufacturing has been an intensive research field in so far as such processes with multiple objectives result in more meaningful solutions. Many works had been aimed at the optimization of polymerization reactors' and processes' performances. One of the first MOO problems was solved for the Nylon 6 reactor by Mitra *et al*. [49]. They utilized a kinetics scheme combined with a batch reactor model. Objectives to minimize were (a) reaction time and (b) undesired product concentration. Constraints implemented were desired monomer conversion and the degree of polymerization. For a solution of a current MOO problem, they used NSGAs, and constraints were handled by penalty functions. Authors varied different GA parameters (e.g. number of generations, crossover probability) to show the stability of obtained Pareto sets because no significant changes were observed. Earlier authors tried to carry out SOO for the same system with Pontryagin's principle; this failed due to some numerical complexity. It was emphasized that NSGA allowed for the overcoming of previous problems and generation of a reasonable set of optimal solutions.

An interesting discovery was found in Bhaskar *et al*. [50]. The authors carried out MOO for a polyethylene terephthalate wiped-film reactor. They chose to minimize the (a) acid and (b) vinyl end group concentration in the polymer product for a better polymer quality. Optimization with NSGA showed that the problem had

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a unique solution instead of a Pareto set. To confirm the results, they carried out the SOO problem for each objective independently; it resulted in the same solution. Later, in another work by Bhaskar *et al*. [51], it was pointed out that the unique solution was dependent on the seed random generator (a number used in computer code to execute randomization). By varying this number, they always obtained different single optimal points. Also they showed that NSGAs didn't obtain an optimal point if more than one decision variable was used. The conclusion was made that NSGAs failed to converge to global optimal solutions and some other search technique is required. Current issues were resolved in Babu *et al*. [52], in which the authors used a multi-objective differential evolution (MODE) for the optimization of the same system. Different MOO cases were considered and MODE converged to a Pareto front in each of them.

Many other similar works for optimization of industrial continuous or batch polymerization processes are made. In general, it can be noted that the main objectives in MOO problems could be:

- maximization of monomer conversion;
- minimization of the concentration of side products or some functional groups; and
- maintainence of quality-related parameters on a desired level (e.g. molecular weight, degree of polymerization).

Some MOO problems include a design stage and significant improvement in the reactor's performance is reported. For example, in the work by Agrawal *et al*. [53] the operation of another type of polyethylene reactor, tubular, was optimized. Two objectives were to maximize monomer conversion and minimize the concentration of side products. The reactor and jacket diameter, and length of reactor zones were included as decision variables. So they carried out optimization of both design-stage and operation-stage optimization. They reported improved results in objectives when compared to the case when design variables are not included into the MOO problem [54].

For MOO problems in polymerization reactors and processes, researchers mentioned significant computational issues such as: to obtain global optimal solutions, large computation time is required. The mathematical models are relatively complex for such processes, because they include mass, heat and momentum balance equations that could include comprehensive equations involving partial derivatives or other intensive mathematical variables involving highly non-linear equations. To carry out MOO using GAs, it is required to perform a number of simulation runs to evaluate objectives for one population, while a MOO search requires a number of generations to obtain convergence to a global optimal Pareto front. All together, it increases computational time up to some hours or even days and hence necessitates the use of supercomputers.

Besides the polymerization processes, there are works made in monomer production. Most commonly used objectives used in these MOO problems are monomer's yield and selectivity. Among the works, there is a group of researchers who optimized styrene production. They carried out various MOOs for different reactor types using different algorithms. Firstly, Yee *et al*. [55] performed two-objective optimization for the operation of adiabatic and steam-injected reactors. The same work was done by Li *et al*. [56], but including reactor design parameters into decision variables. Both used NSGAs with a penalty function approach and obtained smooth Pareto fronts. Babu *et al*. [57] performed a MOO for an adiabatic styrene reactor with the same problem formulation but used a multi-objective differential evolution. They reported a better Pareto front. However, it can be noted that MODE hadn't affected the Pareto front significantly, but there are still improvements in objective values for some MOO cases. Tarafder *et al*. [58] compared performance of three types, single-, double-bed and steam-injected reactors, with NSGA-II in a three-objective problem formulation (maximization of yield and selectivity of styrene plus minimization of heat-exchanger duty). They showed better objective values for the double-bed reactor. It can provide better productivity for styrene with a higher selectivity at the same time.

Table 1: Application of GAs in chemical reactors and processes engineering.

Process/unit	Objectives/constraints	Optimization method	Remarks and comments	Reference
Petroleum processing				

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FCC reactor-regenerator	– maximize gasoline yield – minimize CO % in flue gas constrained by coke content on catalyst – maximize gasoline yield – minimize air feed rate to regenerator constrained by CO % in flue gas The same two objectives plus – minimize air feed rate to regenerator	NSGA-II	The satisfying optimal solution can be chosen from the obtained Pater set by DM.	[41]
	– maximize yield of gasoline – minimize coke percentage on catalyst	NSGA-II-JG	Obtained Pareto set with better distribution and faster convergence than at Kasat *et al.* [41].	[35]
	– maximize gasoline yield – minimize % CO in flue gas constrained by coke content on catalyst The same two objectives plus – minimize air feed rate to regenerator	MOSA	Pareto set is comparable with ones obtained with NSGA-II.	[59]
Naphtha Catalytic Reforming Reactor	– maximize light aromatics yield – Minimize heavy aromatics yield	NAGA	Pareto set obtained which is superior to current unit operation performance.	[42]
Naphtha Catalytic Reformer with Thermally Coupled Fluidized Bed Heat Exchanger	Maximize: – hydrogen production – aromatics production and selectivity – aniline flow rate	Objective sum method, solved by differential evolution	Reactor performance compared to conventional naphtha reformer.	[43]

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	Maximize: – hydrogen production – aromatics production – nitrobenzene conversion – aniline flow rate		Single optimal solution obtained which allowed improving reactors performance.	[44]
Spherical (S) and Tubular Membrane Naphtha (M) Reforming Reactor	Maximize: – hydrogen flow rate – aromatics flow rate Two reactor arrangements in series – SMS and SMM – are investigated.		Both arrangements perform similarly but SMS has some design advantages and proposed as better one.	[45]
Naphtha Pyrolysis	Maximize yield of: – ethylene – propylene	MOPDE-CES, NSGA-II	Optimal solutions obtained. MOPDE-CES performs slightly better.	[60]
HVGO Hydrocracker	3 MOO cases: – maximize kerosene flow rate – minimize hydrogen flow rate – maximize diesel flow rate – minimize hydrogen flow rate – minimize light products flow rate – maximize heavy products flow rate constrained by inlet temperature at hydrocracker and outlet temperature at beds, liquid velocity rate, feed conversion	Real-coded NSGA-II with simulated binary crossover	Pareto set obtained for all cases. Wide range of equally optimal solution are presented for DM.	[61]

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	2 MOO cases: – maximize the sum of all desired products – maximize the sum of heavy desired products constrained by inlet temperature at hydrocracker and outlet temperature at beds, feed conversion	GA with artificial neural network model	Shown possibility to improve reactors performance up to 16 %.	[62]
Paraffin dehydrogenation reactor of LAB plant	For process product (olefins) maximize: – production rate – selectivity	NSGA-II with crowding tournament selection operator	Dynamic optimization was carried out. Shift of Pareto from is shown due to catalyst deactivation.	[63]
Industrial Steam Reformer	For a required hydrogen rate production – minimize methane feed – maximize CO at reactor's outflow constrained by maximum tube wall temperature	NSGA with penalty function approach	The satisfying optimal solution can be chosen from obtained Pater set by DM.	[46]
	For a step disturbances of (a) methane feed (b) temperature minimize deviation from steady-state values for – hydrogen production – steam production	NSGA-II	The satisfying optimal solution can be chosen from obtained Pater set by DM.	[47]
	Same as Nandasana *et al.* [47] but only for case (a) step decrease in feed	MOSA-JG, MOSA-aJD	Comparable Pereto set to the one obtained using NSGA-II.	[64]
	– maximize methane conversion – Maintain desired ratios for H_2/CO_2 and H_2/CO MOO problem solved for dynamic model.	GA	Authors used different operating conditions and transition between them. Final problem is formulated in form of singleobjective function.	[65]

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Autothermal reformer	– maximize methane conversion – maximize CO selectivity – minimize CO_2 feed rate	NSGA-II	Pareto set is obtained. Among it, authors chose one point with H_2/CO ratio = 1 as an optimal operating point.	[66]
Methane and autothermal steam reformers	For two arrangements of reactors – in parallel and in series: – maximize production of syngas – minimize furnace fuel consumption	NSGA-II	Parallel configuration is better for syngas. Arrangement in series is superior for lower fuel consumptions and CO_2 release.	[48]
Polymers synthesis				
Nylon 6 semibatch reactor	For a required monomer conversion minimize: – dimensionless reaction time – dimensionless side product concentration constrained by required values for average polymer length	NSGA with penalty function approach	Superior approach comparing to previous attempt to carry out MOO.	[49]
	Cases 1 and 2: same as Mitra *et al.* [49] but different decision variables Case 2: – Same as case 2 – maximize monomer conversion	NSGA-II-aJG, MOSA-aJG	NSGA-II-aJG has a better distribution of individuals in Pareto front.	[67]
Sheet-molding for poly(methyl methacrylate)	– maximize monomer conversion – minimize length of film reactor constrained by the end value of polymer molecular weight	NSGA with penalty function approach	The satisfying optimal solution can be chosen from obtained Pater set by DM.	[68]
Poly-ethylene wiped-Film reactor	Minimize: – acid – vinyl groups in the product constrained by desired degree of polymerization	NSGA with penalty function approach	Single optimal solution.	[50]

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	Same as Bhaskar *et al.* [50] plus additional constraint for di-ethylene glycol group concentration	NSGA with penalty function approach	Fails to converge the optimum solution for multiple decision variables.	[51]
	Same as Bhaskar *et al.* [50]	MODE with penalty function approach	Pareto set obtained in contrast to Bhaskar *et al.* [50].	[52]
Isothermal polystyrene reactor	– maximize styrene conversion – minimize remaining initiator concentration in final product	Authors' version of MOGA (includes real-coded variables, elitism, niche count) with fuzzy penalty function approach	The satisfying optimal solution can be chosen from obtained Pater set by DM.	[69]
Styrene emulsion homopolymerization	– maximize styrene conversion minimize deviations from desired values for: – Polymer average molecular weight – Number of particles per liter	Diploid GA followed by decision support system	Decision support system narrowed the Pareto set.	[70, 71]
	– minimize operating cost of reactor – minimize integral square difference of average molecular weight from its desired value	Mixed-integer dynamic optimization, ε-constraint approach	Optimization for design and control is carried out.	[72]
Epoxy polymerization	For polymer product: – maximize molecular weight – minimize reaction time Constrained by minimum desired molecular weight and maximum desired polydispersity index	NSGA-II with crowding tournament selection operator	Pareto set obtained for each case and the satisfying optimal solution can be chosen from obtained Pater set by DM. It is found that for molecular weight vs. polydispersity index, set is non-convex. Binary and real coded NSGA-II performs similarly.	[73]

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Case 1: – maximize polymer molecular weight – minimize polymer polydispersity index Case 2: – maximize concentration of species with glycidyl ether groups at both ends – minimize polymer chain propagation Case 3: – Same as case 2 – + minimize total addition of NaOH	NSGA-II with crowding tournament selection operator	[74]
Case 1: – maximize concentration of particular species – minimize polymer chain propagation – minimize reaction time Case 2: – minimize total addition of NaOH – + last 2 objectives from case 1	Real-coded NSGA-II	[75]
3 MOO problems for following objectives: – maximize polymer's average molecular weight – minimize polydispersity index – minimize reaction time	NSGA-II, Real-coded NSGA-II	[76]

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Styrene and acrylonitrile copolymerization in semi-batch reactor	Case 1: – maximize monomer conversion – minimize polydispersity index of final product Case 2: – Same as case 1 – minimize presence of unreacted monomer at reactor	NSGA-II with crowding tournament selection operator	Pareto set obtained in both cases. Process control policies are defined.	[77]
	Minimize deviations from desired: – Copolymer molecular weight – Copolymer composition	Differential evolution	Dynamic optimization is carried out.	[78]
Poly-ethylene tubular reactor	For poly-ethylene: – maximize monomer conversion – minimize side products constrained by desired range for product molecular weight and maximum process temperature	NSGA and JD adaptations, NSGA-II and JD adaptations with penalty function approach	All algorithms provide similar, but NSGA-II converges faster.	[54]
	Two MOO problems: Same as Agrawal *et al.* [53, 54] Same as Agrawal *et al.* [54] +1 objective to minimize compressor operating cost * Design parameters as reactor length and diameter were included as decision variables.	NSGA-II and JD adaptations with: – Penalty function approach – Constraint dominance approach	Improved reactor performance comparing to operation MOO only. Constraint-dominance approach is better than penalty function.	[53]
Polysiloxane synthesis	– maximize monomer conversion – minimize the difference between real and desired molecular weight of polymer	NSGA-II combined neural network	Improved performance of method comparing to NSGA-II.	[79]

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Styrene and butyl acrylate emulsion copolymerization reactor	– maximize monomer conversion – deviation from desired glass temperature profile	Evolutionary algorithm followed by multi-attributive utility theory	A single solution was chosen from obtained Pareto set with decision support system.	[80]
Adiabatic and Steam-Injected Styrene Reactors	4 MOO problems: for styrene maximize either two of three objectives or all of them: – productivity – selectivity – yield constrained by steam feed rate and inlet streams temperature	NSGA with penalty function approach	The satisfying optimal solution can be chosen from obtained Pater set by DM.	[81] [55]
	For styrene maximize: – productivity – selectivity constrained by steam feed rate and inlet streams temperature plus exit pressure for steam-injected reactor * Design parameters as reactor length and diameter were included as decision variables.	NSGA with penalty function approach	The satisfying optimal solution can be chosen from obtained Pater set by DM.	[56]
Adiabatic Styrene Reactor	Same as Yee *et al.* [55]	MODE with penalty function approach	MODE provides improved Pareto set comparing to the one from Yee *et al.* [55].	[57]
	2 MOO problems: – maximize styrene production – minimize undesired products for new and deactivated catalyst	Tabu Search, GA	Better objective values as well as less computational time for Tabu Search.	[82]
	Same as Yee *et al.* [55]	Author's Hybrid-MODE	Proposed algorithm compared with other well-known MOEA and showed better performance.	[83]

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Ethylene Reactor	For ethylene maximize: – flow rate – conversion – selectivity constrained by reactor pressure and temperature	NSGA-II with crowding tournament selection operator	Feed temperature and reactor length are mostly affect Pareto optimal solutions.	[84]
Single-bed, steam-injected and double-bed styrene reactors	For styrene: – maximize productivity – maximize selectivity – heat duty of heat exchanger constrained by inlet streams temperatures, reactor pressure * Design parameters such as reactor length and diameter were included as decision variables.	NSGA-II with crowding tournament selection operator	Double-bed reactor has higher productivity.	[58]
Adiabatic and steam-injected styrene reactor	Same as at Yee *et al.* [55]	MODE with penalty function approach	Obtained Pareto set has better objective values than the one with NSGA.	[85]
Hydrogen production				
Hydrogen plant (natural gas operating)	Maximize production of: – hydrogen – steam constrained by maximum tube wall temperature, H_2O/H_2 ratio and some other limitations for equipment operating condition	NSGA with penalty function approach	The satisfying optimal solution can be chosen from obtained Pater set by DM.	[86]
	Same as at Rajesh *et al.* [86] plus minimize heat duty of reformer tubes	NSGA with penalty function approach	More practical information about Pareto front for three-objective optimization problem.	[87]
	Same as at Oh *et al.* [87]	NSGA with penalty function approach	Pareto set is affected by origin of feed (comparing to Oh *et al.* [87]).	[88]
Hydrogen plant with absorber and methanator instead of PSA unit	Same as at Rajesh *et al.* [86]	NSGA with penalty function approach	The satisfying optimal solution can be chosen from obtained Pater set by DM.	[89]
Other processes an reactors				

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Purified terephtalic acid oxidation	4 MOO cases: – minimize concentration of intermediate product in outflow – maximize feed rate to reactor with different number of decision variables	NAGA	Pareto sets obtained for each case. The more decision variables are taken into account the better objectives are reached.	[90]
Syngas production using CO_2 reforming and natural gas (methane) partial oxidation	– maximize methane conversion – maximize total selectivity for CO production – keep H_2/CO molar ratio around required value constrained by O_2/CH_4 molar ratio, gas stream velocity	Real-coded NSGA	Empirical process model was utilized. Better objective values are reported comparing with previous SOO.	[91]
Phthalic anhydride catalytic reactor	For 2 different reactor arrangements: – maximize product yield – minimize catalyst mass	NSGA-II-aJG, Guided NSGA-II-aJG with penalty function approach	Guided NSGA-II needs proper choice of genetic parameters but provides faster convergence to Pareto.	[37]
Membrane methanol synthesis reactor Membrane hydrogen synthesis reactor	– maximize desired product rate – minimize feed rate – minimize exergy loss in reactor	NSGA-II	Pareto set for hydrogen reactor is very clear and readable while the one for methanol has scatter data.	[92]
Oxidative coupling of methane in simulated moving bed reactor	– maximize methane conversion – maximize selectivity for ethane and ethylene operation and design MOO are carried out.	NSGA-II-JG	Pareto-optimal sets are provided.	[93]
	Same as at Kundu *et al.* [93]	NSGA-II-JG	MOO problem is similar to [93], but reactor configuration is different.	[94]

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Porous ceramic membrane reactor for oxidative coupling of methane	3 objectives are: – maximize methane conversion – maximize selectivity for ethane and ethylene – maximize yield for ethane and ethylene and 2 MOO cases for operation stage and 2 MOO cases for design case are solved for two out of three objectives	NSGA-II-aJG	Reactor length and diameter were included into MOO on design stage. MOO of design stage showed significant improvement in objectives.	[95]
Thermal cracker for LPG	Operation and design MOO problems using 2 or 3 objectives from list are solved: maximize: – ethylene production – propylene production – ethylene selectivity – furnace run length minimize: – severity – heat duty	NSGA-II-aJG	Pareto set obtained for each MOO case. Three-objective problems provide better range of solutions. Design optimization provides better objective values.	[96, 97]
Autothermal membrane reactor for simultaneous dehydrogenation of ethylbenzene to styrene with the hydrogenation of nitrobenzene to aniline	– maximize styrene yield – maximize nitrobenzene conversion Optimization problem included design variables	Normalized normal constraint and normal boundary intersection methods	Both methods provided the same Pareto sets.	[98]

4.10 Conclusions

The multi-objective optimization approach is superior to classical single-objective optimizations. It can take into account more than one objective; this is very important when objectives conflict with one another. Reactors and processes systems in chemical engineering include many parameters (qualitative or quantitative parameters that characterize the process performance), which cannot be improved without any detriment to others. So the application of MOO can play a vital role in making process operation improvements. In summary, the general ideas of MOO techniques as well as the advantages in applying the concept of MOO in the design and operation of chemical reactors and processes engineering are reported.

– MOO is based on the concept of Pareto optimality. In contrast with SOO, no single optimal solution but a set of optimal solution results are more meaningful. This set is called a Pareto set. None of the solutions in a Pareto set is better than any others in the set.

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– Various MOO methods are discussed that helps in search of solutions in the form of a Pareto set. There is a variety of these methods available. Each has its own advantages and disadvantages. Researchers are free to choose any of them depending on the particular problem he/she is trying to solve.

– In the field of chemical reactors and processes engineering, a group of stochastic optimization methods, called genetic algorithms, showed robustness in finding Pareto-optimal solutions.

– Genetic algorithms are not based on a deterministic mechanism of search, and require no extra *a priori* knowledge (like weighting information of preference order) about MOO of conflicting objectives. Also, GAs work with a population of solutions simultaneously, not a single one; hence they search a global space for optimum solutions.

– Many of the reported work carried out by researchers shows the significance of MOO in chemical engineering. It can be done at the operation stage level, because many industrial reactors operate in non-optimal regimes and there's still room for improvements. It's also useful for the design stage, which can significantly improve a reactor/system performance when designing reactors.

– Among GAs, there are some more advanced algorithms that are able to converge to a Pareto front in less computation time while providing better distribution of solutions. Researchers should take it into account when applying them to MOO problem.

– A majority of Pareto fronts in chemical engineering are convex in nature; however, it's not an absolute rule.

– Many problems considered only 2, or at most 3, objectives. Researchers are trying to pick out more important ones based on their knowledge about particular systems. Also, it is more difficult to visualize and analyze results if more than 3 objective functions are chosen.

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