

Differential Evolution for Multiobjective Optimization of Process Design Problems

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Abstract: Optimization is a highly important area in chemical engineering, particularly for process design that is generally formulated as a mixed and non-linear problem with several competing objectives. A way to tackle the problem is to couple multiobjective optimization based on evolutionary algorithms with a process simulator. This situation may yet lead to prohibitive computational time as the number of objectives increases. In this paper, the potential of multiobjective differential evolution (MODE) is tested with three different stopping criteria. The performance of MODE is compared with the results obtained with a variant of NSGA II. The performance metric is based on the number of evaluations used to get the Pareto front. The results show that the combination of an efficient algorithm and the stopping criterion helps to reduce the optimization time but its choice may affect the results. As far as multiobjective is concerned, it must be emphasized that the final solution is the result of compromise that the decision maker must be aware.

1 INTRODUCTION

Process design is a key activity in the chemical engineering field for implementing new technologies, creating new facilities, or retrofitting existing processes. If the traditional design approach incorporates economic objectives, process systems design has come to include more performance measures, such as environment, safety, controllability, and flexibility. This kind of problems can be generally modelled as mixed integer nonlinear programming (MINLP) formulations, involving continuous and integer variables. This class of mathematical problems generally involves non-convexities, which are related to the problem formulation concerning both the objective function(s) and/or the set of constraints. The inherent combinatorial nature of the problem contributes to its complexity. In that context, evolutionary algorithms (EAs) have received a lot of attention for solving nonlinear multimodal problems (Angira and Babu, 2006). They are also particularly attractive to capture the multiobjective nature of the criteria. Among the methods that have reported in the dedicated literature, multiobjective optimization (MOO) (Rangiah, 2009) and particularly

evolutionary algorithms constitute a promising approach to tackle the problem.

The early design stage implies the evaluation of the various alternatives that can be used to produce a chemical product involving several reaction routes with various types of equipment and their corresponding operating conditions. The importance of early design activities has been addressed in several recent studies. The problem is generally solved by use of a process simulator for flowsheet generation such Aspen ("Aspen One® - AspenTech," 2013), Hysis ("Aspen HYSYS® - AspenTech," 2013), Prosim ("PROSIM," 2013).

If the computational time required for simulation is quite acceptable (from several seconds to several minutes for large size problems), the situation may be quite different when performing optimization where the various objectives must be evaluated many times by successive use of the process simulator. It must be emphasized that multiobjective optimization does not lead to a single ideal solution but to a set of compromise solutions (Jones et al., 2002) that are generally represented through a Pareto front as far as the objective functions are considered.

Problems such as the optimization of the process of hydrodealkylation (HDA) of toluene, to produce benzene were investigated previously (Ouattara et

al., 2012) involving various objective functions based on economic and ecological criteria evaluated by coupling two simulators for chemical process and utility requirement. Every evaluation involves a call to the support software tools that makes the optimization task quite long. Another example is the selection of the synthesis strategy for a chemical plant described by Grossmann (Papoulias and Grossmann, 1983). The superstructure considers the chemical and utility plant as the heat recovery network. The objectives are to determine the configuration of the plant, the heat exchanger network and utility system that allows maximizing the annual profit. Other examples can be mentioned such as the supply chain management problem presented in (Kallrath, 2000) as a multi-site, multi-product, multi-period production/distribution network planning system with the objective of finding the best production schedule satisfying a given demand.

Among multiobjective evolutionary approaches, Genetic Algorithms (GAs) constitute a quite popular method used in engineering field, particularly in the chemical engineering community (Abbass et al., 2001). One of the most efficient genetic algorithms is NSGA II Non-dominated Sorting Genetic Algorithm (Deb et al., 2002) an upgrade version of NSGA which estimates the density of solutions surrounding a particular one, in order to perform a scanning of the solution space.

The design optimization time obviously depends on the number of the successive evaluations of the possible solutions by use of the process simulator. In that context, the formulation of an effective criterion is necessary in the case of the multiobjective optimization problem as judging the advance of the optimization. If the selection of an appropriate criterion has been identified as one of the fundamental topics, it must be highlighted that this issue has not been solved properly.

The objective of this work is twofold: first, the potential of Differential Evolution (DE) is investigated since DE has been successful in the solution of a variety of continuous single-objective optimization problems in which it has shown great robustness and a very fast convergence. Recently, there have been successful proposals to extend DE to MOO (Robič and Filipič, 2005). A multi-objective differential evolution algorithm was thus implemented. The second objective is to evaluate different stopping criteria for reducing the number of evaluations. For this purpose, some benchmark problems and a chemical engineering problem are tested.

This paper is divided into 5 sections. Section 2 is devoted to main concepts of differential evolution. Section 3 describes the solution strategy. Section 4 discusses the results obtained with test problems. Section 5 concerns the application to a small-size structural problem for process design. Finally, conclusions and perspectives are proposed.

2 DIFFERENTIAL EVOLUTION (DE)

Differential Evolution (DE) is an evolutionary algorithm proposed by Price (Price, 1996) using vectors to perturb the best solution found so far together with mutation and crossover. It needs three parameters, i.e., population size NP , scaling constant F and crossover constant CR .

The details on DE algorithm, various strategies of DE and wide range of applications in various engineering areas are well documented in literature (Angira and Babu, 2006)(Onwubolu and Babu, 2004). Only the principles are presented here for the sake of brevity.

The procedure is rather simple. The first step is to initialize the population Pop for every variable in the dimension D and evaluate the fitness of each individual j within the boundary constraints (upper and lower bounds H and L , respectively), such as:

$$Pop_{ij} = L + (H - L)rand_{ij}[0,1], i = 1, \dots, D; j = 1, \dots, NP \quad (1)$$

Each iteration consists in 4 steps. First, three individuals of the population are randomly selected (r_1, r_2, r_3); they must be mutually different and also different of the current vector j . Secondly, a trial vector x is created according to equation (2), where $rand_{ij}[0,1]$ is a randomly generated number and Rnd is a randomly selected variable.

$$x_i = \begin{cases} x_{i,r_3} + F(x_{i,r_1} - x_{i,r_2}) & \text{if } (rand_{ij}[0,1] < Cr) \vee (Rnd = i) \\ x_{ij} & \text{otherwise} \end{cases} \quad (2)$$

Step 3 checks the boundary constraints; if a value is out of the boundary zone, it is calculated again according to:

$$\text{if } (x_i \notin [L, H]) \ x_i = L + (H - L)rand_i[0,1]. \quad (3)$$

Finally, if the trial vector is inferior or equal to the current one, the trial individual replaces the current individual.

Some guidelines for the use of DE are proposed in (Storn, 1996):

- At initialization step, the population should be

spread as much as possible over the objective function surface.

- Most often, the crossover probability CR ($\in [0, 1]$) must be considerably lower than 1. If no convergence can be achieved, a value of CR within $[0.8, 1]$ is yet recommended
- For many applications, a size of the population corresponding to 10 times the size of the problem D ($NP = 10D$) is a good choice. F is usually chosen within the interval $[0.5, 1]$.

Some differences between DE and GA (Abbass et al., 2001) can be highlighted:

- In GAs, crossover is carried out between two parents and the child is a recombination of both of them, while in DE, three parents are selected and the child is only the perturbation of one of them.
- The new child only replaces a randomly selected vector of the population when it is better. In GA, the children replace the parents with some probability regardless of their fitness.

2.1 Stopping Criterion

As mentioned in the motivation of this work, the stopping criterion is of major importance to guarantee that the solution (or the set of solutions) obtained so far is of acceptable quality regarding the numerical effort. Various scenarios can be used among others (Martí et al., 2007):

- the solution yielded so far is satisfactory;
- the method is able to produce a solution : it is yet not satisfactory but a better one will not be produced;
- the method is unable to “converge” to any solution;
- there is no progress in the search of a new solution.

3 SOLUTION STRATEGY

3.1 Principles

The algorithm used is the one suggested by Price (Price, 1996) that was adapted for considering mixed variables and a multiobjective formulation. By lack of place, a major attention is only paid to the stopping criterion in what follows.

The binary variables are taken into account using the strategy of Angira (Angira and Babu, 2006), that means that the variable is handled as a continuous

one, within the interval (Feoktistov, 2006) with a rounded value (Feoktistov, 2006). Every variable that is modified during the optimization process must be within its definition domain; otherwise, it is initialized again.

The violation of constraints is calculated and used in the adaptation comparison procedure according to Deb’s criterion, that means that a vector A dominates B if one of the next conditions is achieved (Deb et al., 2002):

- A is feasible and B not;
- A and B are not feasible but the violation of the constraints is lower in A than in B;
- A and B are feasible but A dominates B.

3.2 MGMB

The MGMB criterion (from the initials of the authors (Martí et al., 2007)) is based on the comparison of the set of non-dominated solutions of two iterations. A progress indicator (s_t) is to be calculated indicating or not an evolution of the population. For example, a value of s_t equal to 1 means that the last population is better than the previous one. A value of s_t equal to 0, means that there is no progress and a value of s_t equal to -1 is the sign of deterioration of the population. A correction step K_t is considered to take into account the influence of the changes.

3.3 Consolidation Ratio (CoR)

This is a convergence metric that can be used as a stopping criterion. The consolidation ratio is the fraction of the population at the generation $i - \Delta$ (Δ represents a kind of observation step) that has evolved up to the current generation i .

This is calculated as the ratio of the number of non-dominated individuals (ND) in the generation $i - \Delta$ present in the generation i and the non-dominated of the last generation (i), expressed as:

$$CoR = \frac{ND_{i-\Delta}}{ND_i} \quad (4)$$

In the early stages of the algorithm, a large fraction of non-dominated will not remain in the last population that will result in a low value for CoR, while the quantity of non-dominated individuals after several generations that will remain in the population will be higher, leading to a CoR ratio close to 1 (no changes of non-dominated vectors).

3.4 Improvement Ratio (IR)

This ratio represents the proportion of the population $i - \Delta$ dominated by the population i of size n_i , as expressed by:

$$IR = D_{i-\Delta}/n_i \quad (5)$$

The initial value of this ratio is equal to unity, which means that every solution is dominated by the latest population, while when convergence is achieved this value is equal to zero.

3.5 Final Selection with TOPSIS

The final selection process is made using a multicriteria decision-making process that takes into account the optimal alternatives found in the Pareto front. These alternatives are found to be non-dominated solutions near optimal value, and although the decision maker may use judgment to make the final selection from the alternatives, a formal method based on TOPSIS (Technique for Order of Preference by Similarity to Ideal Solution) was adopted (Lai et al., 1994); (Ren et al., 2010). This method is based on the idea of choosing the best alternative solution from a set by analyzing the shortest geometric distance from the positive ideal solution and the longest distance from the negative ideal solution. It also requires weights to be assigned per criterion and normalizes the information, so that the various alternatives are ranked. Although other ranking and classification methods exist, TOPSIS has proven its efficiency in the final alternative selection process obtained through GA (Gomez et al., 2010) and is used here after MODE process. The same weight was allocated to each criterion in the experimental study. The approach for each stopping criterion will be tested based on the solution that obtained the top rank by TOPSIS.

4 VALIDATION

The test problems selected to evaluate the performance of the algorithm are the classical SRN and TNK problems used in previous works (Deb et al., 2002). The formulation of the two problems is presented in Table 2 as well as the Pareto fronts of SRN and TNK. First, to validate the algorithm, the classical DE algorithm was used without any specific stopping criterion (the algorithm stops when the maximum number of generation is reached) and the results were compared with the solutions

obtained by previous researchers with other algorithms. The parameters used were CR=0.6, F=0.8, NP=200 and 100 generations. They can be visualized in Fig. 1 and 2 and are in agreement with the results obtained with deterministic methods.

Then, the three stopping criteria are considered for DE i.e., the so-called MGMB (Martí et al., 2007), consolidation ratio (Goel and Stander, 2010) and improvement ratio (Goel and Stander, 2010) in combination with the maximum number of generations.

The DE procedure is compared with a variant of NSGA II developed for mixed problems and implemented in the Multigen environment (Gomez et al., 2010). The stopping criterion proposed in Multigen (in addition to the maximum number of generations) consists in comparing the Pareto fronts associated with non-dominated solutions for populations n and $n + p$, where the period $p \in [10, 20, 30, 40, 50]$ for example. If the union of the two fronts provides a single non dominated front, the procedure stops; else the iterations continue.

Table 1: Problem formulation for the test functions.

SRN	TKN
$\text{Min } f_1(x) = (x_1 - 2)^2 + (x_2 - 1)^2 + 2$	$\text{Min } f_1(x) = x_1$
$\text{Min } f_2(x) = 9x_1 - (x_2 - 1)^2$	$\text{Min } f_2(x) = x_2$
$g_1(x) = x_1^2 + x_2^2 \leq 225$	$g_1(x) = -x_1^2 - x_2^2 + 1 + 0.1 \cos(16 \tan^{-1}(x_1/x_2)) \leq 0$
$g_2 = x_1 - 3x_2 \leq -10$	$g_2(x) = (x_1 - 0.5)^2 + (x_2 - 0.5)^2 \leq 0.5$
$x \in [-20, 20]$	$x \in [0, \pi]$

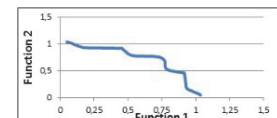
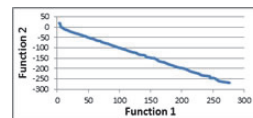


Figure 1: Pareto front of the test problem SRN.

Figure 2: Pareto front of the test problem TNK.

Three scenarios for DE and one for NSGA-II are tested as shown in Table 2. The period represents the time of observation and application of the stopping criterion. Every problem is analyzed relative to the number of evaluations performed for each stopping criterion and procedure. The solutions obtained after TOPSIS application are also analyzed which can be viewed as another validation. The solutions concern

both the values of the objective functions and the associated variables.

Table 2: Scenarios for DE and NSGA-II.

	DE Test 1	DE Test 2	DE Test 3	NSGA II
Individuals	100	100	100	100
Maximum number of generations	200	200	200	200
CR	1	0.6	0.4	0.9
F	0.8	0.8	0.8	0.5 (mutation)
Period	10	10	5	-

By lack of place, the Pareto front obtained for each problem is not presented here. All the fronts exhibit similar behaviors as previously seen in Fig. 1 and 2. It must be said that the curves are overlaid in the domain with common intersection each other.

For SRN problem (see Table 1), the solutions obtained by DE-TOPSIS exhibit a similar behavior both for criteria and variables. The order of magnitude of criteria and variables is quite different with NSGA-II. It must be emphasized that for NSGA II, the algorithm ends because the maximum number of generations is reached. Regarding the objective functions, the stopping criteria IR and CoR require yet a higher number of evaluations (Figure 3) than MGMB.

For TNK problem (see Table 1), the order of magnitude of the objective functions is quite similar, in fact all the selected solutions are non-dominated between them. Considering the number of evaluations, it is interesting to see that the MGMB requires around 9 times lower evaluations than the other criteria, which can be of practical importance

in solving real problems (Figure 4). Considering the homogeneity of the selected solutions obtained after DE-TOPSIS, IR shows almost no difference, while CoR and MGMB have a larger deviation. This can be attributed to scattered points in the Pareto front obtained for each test, thus giving different ranking after application of TOPSIS method.

5 APPLICATION TO A STRUCTURAL DESIGN PROBLEM

This problem is a bicriteria one proposed by Papalexandri and Dimkou (Papalexandri and Dimkou, 1998). It consists of 3 continuous variables, 3 binary variables and two objective functions. The formulation can be expressed as follows:

$$\text{Min } f_1(x, y) = x_1^2 - x_2 + x_3 + 3y_1 + 2y_2 + y_3 \tag{6}$$

$$\text{Min } f_2(x, y) = 2x_1^2 + x_3^2 - 3x_1 + x_2 - 2y_1 + y_2 - 2y_3 \tag{7}$$

$$g_1(x, y) = -3x_1 + x_2 - x_3 - 2y_1 \geq 0 \tag{8}$$

$$g_2(x, y) = -4x_1^2 - 2x_1 - x_2 - x_3 + 40 - y_1 - 7y_2 \geq 0 \tag{9}$$

$$g_3(x, y) = x_1 + 2x_2 - 3x_3 - 7y_3 \geq 0 \tag{10}$$

$$g_4(x, y) = x_1 + 10 - 12y_1 \geq 0 \tag{11}$$

$$g_5(x, y) = -x_1 + 10 + 2y_1 \geq 0 \tag{12}$$

Table 3: Selected solutions for SRN and TNK problem using DE-TOPSIS.

	SRN				TNK			
	x_1	x_2	f_1	f_2	x_1	x_2	f_1	f_2
NSGA-II	0,0282	18,4389	310,003	-303,861	0,043	1,039	0,043	1,039
IR Test 1	-2,418	-11,666	181,939	-182,183	1,029	0,063	1,029	0,063
IR Test 2	-2,539	-12,499	204,821	-205,07	1,006	0,088	1,006	0,088
IR Test 3	-2,924	14,1161	198,274	-198,344	1,022	0,072	1,022	0,072
CoR Test 1	-2,288	-8,6635	113,773	-113,978	1,006	0,088	1,006	0,088
CoR Test 2	-2,165	-12,371	198,117	-198,254	0,957	0,138	0,957	0,138
CoR Test 3	-2,351	-12,292	197,614	-197,842	0,089	1,004	0,089	1,004
MGMB Test 1	-2,066	13,1749	166,762	-166,824	0,108	1,011	0,108	1,011
MGMB Test 2	-2,287	14,1367	192,948	-193,152	0,068	1,026	0,068	1,026
MGMB Test 3	-3,176	-12,307	205,862	-205,656	0,066	1,042	0,066	1,042

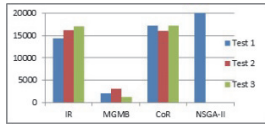


Figure 3: Number of evaluations for SRN problem.

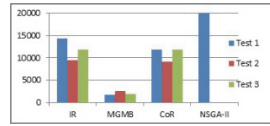


Figure 4: Number of evaluations for TNK problem.

$$g_6(x, y) = x_2 + 20 - y_2 \geq 0 \quad (13)$$

$$g_7(x, y) = -x_2 + 40 + y_2 \geq 0 \quad (14)$$

$$g_8(x, y) = x_3 + 17 - y_3 \geq 0 \quad (15)$$

$$g_9(x, y) = -x_3 + 25 + y_3 \geq 0 \quad (16)$$

$$x_i \in [-100, 100] \quad (17)$$

$$y_i \in [0, 1] \quad (18)$$

For the three stopping criteria, the previous conditions were applied (see Table 2). A similar analysis as the one previously adopted for SRN and TNK is carried out.

For the Improvement Ratio (Fig. 13) all the runs exhibit similar results and the slight discrepancy that is observed can be attributed to the different choice in parameter settings.

For the MGMB criterion (Fig. 14) the behavior is quite similar for all tests, the best performance being obtained by test 3.

For the Consolidation Ratio (Fig. 15) the performance of the three tests is quite similar, meaning that this criterion leads to quasi-identical results whatever the intrinsic parameters of the procedure.

Regarding the number of evaluations of the objective functions (Fig. 16), the stopping criterion MGMB leads to the best performance once more. A

slight difference is observed between IR and CoR, with a lower number of evaluations than NSGA-II.

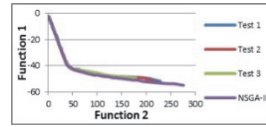


Figure 5: Pareto front with Improvement Ratio as stopping criterion.

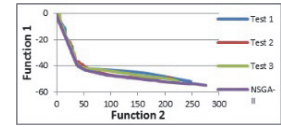


Figure 6: Pareto front with MGMB as stopping criterion.

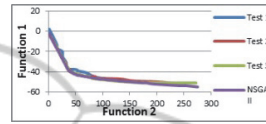


Figure 7: Front de Pareto using Consolidation Ratio as stopping criterion.



Figure 8: Number of evaluations for every stopping criterion.

Table 4) shows that significant differences in solutions are observed. For IR, CoR and MGMB Test 1 and 2, the results for function f_1 are better than those proposed by NSGA-II. Such a situation never occurs for f_2 since they are out-performed by the NSGA-II. Test 2 provides consistent results for all criteria, so the configuration $CR=0.6$ and $F=0.8$, with a period of 10 generations seems the more appropriate for this problem. As far as the number of evaluations is concerned, MGMB is more performing. Yet, if the evaluation functions lead to similar performances, the corresponding set of TOPSIS analysis variables is not the same. The final choice of the decision maker may also consider the difficulty of implementation of a solution over another one as an effective lever.

Table 4: Selected solutions for SRN and TNK problem using DE-TOPSIS for the small-design problem.

	x_1	x_2	x_3	y_1	y_2	y_3	f_2	f_1
NSGA-II	0,0919	39,9759	-1,7991	0	0	0	42,9538	-41,7666
IR Test 1	0,1980	36,4077	-0,6076	0	0	1	34,2613	-35,9761
IR Test 2	0,1969	37,6330	-0,0376	0	0	1	35,1213	-36,6318
IR Test 3	0,4251	35,4294	-0,9154	0	0	0	35,3535	-36,1641
CoR Test 1	-0,0011	40,1225	-1,2869	0	0	1	39,7819	-40,4093
CoR Test 2	0,1405	36,7248	-0,3565	0	0	1	34,4699	-36,0615
CoR Test 3	0,2955	36,8305	-0,4736	0	0	1	34,3429	-36,2167
MGMB Test 1	0,2727	39,4125	-1,3556	0	0	1	38,5809	-39,6938
MGMB Test 2	0,9297	35,2025	-2,7510	0	0	0	35,3495	-36,0356
MGMB Test 3	-0,4732	10,8265	-0,8724	0	0	1	49,3434	-41,3825

6 CONCLUSIONS AND PERSPECTIVES

A differential evolution algorithm with several stopping criteria was developed. Its performance was compared with the results obtained by a variant of NSGA II implemented in previous works. Results show that, every proposed stopping criterion obtained similar results as done by NSGA-II. But, the use of the MGMB criterion implies a lower number of evaluations as compared with IR and CoR. Nevertheless, no stopping criterion is the panacea. Its choice must be a compromise between the required gain and the computational effort. This study will now be applied to a large size chemical engineering design problem which involves the evaluation of every proposed solution with a simulator. Even if MGMB appears to be a good candidate, its robustness must be now investigated as far as multiple variable-mapping is concerned.

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