OPTIMIZATION OF SOME CHEMICAL PROCESSES USING DIFFERENTIAL EVOLUTION (DE) ALGORITHM

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Abstract:Differential Evolution (DE) algorithm is a new heuristic approach mainly having three advantages; finding the true global minimum regardless of the initial parameter values, fast convergence, and using few control parameters. The biggest advantage of the differential evolution approach over other non-traditional method approach is its stability. DE algorithm is a population based algorithm like genetic algorithms using similar operators; crossover, mutation and selection. Differential evolution algorithm can be easily applied to a wide variety of real valued problems despite noisy, multimodal, multidimensional spaces which usually makes the problems very difficult for optimization. Differential evolution becomes impressive because of the parameters crossover ratio (CR) and mutation factor (F) do not require the same tuning which is necessary in many other Evolutionary Algorithms. In the present study, DE has been used to solve the various chemical engineering problems from the literature. We have compared the performance of DE algorithm to that of some other well-known versions conventional and non-conventional optimization methods. From the simulation results, it was observed that the convergence speed of DE is significantly better than the other techniques. Therefore, DE algorithm seems to be a promising approach for engineering optimization problems.

***Keywords* - Optimization, Differential Evolution, Genetic Algorithms, Evolutionary Algorithms.**

I. INTRODUCTION

Optimization plays very important role in the design, planning and operation of chemical processes. Optimization refers to finding one or more feasible solutions, which corresponds to extreme values of one or more objectives. The need for finding such optimal solutions in a problem comes mostly from the extreme purpose of either designing a solution for minimum possible cost of fabrication, or for maximum possible reliability, or others. Because of such extreme properties of optimal solutions, optimization methods are of great importance in practice, particularly in engineering design, scientific experiment and business decision making. More recently, a new evolutionary computation technique, called differential evolution (DE) algorithm, has been proposed and introduced [1, 7-11]. Over the last decade, evolution algorithms have been extensively used in various problem domains and succeeded in effectively finding the near optimal solutions. Evolutionary optimization techniques have been used to solve chemical process optimization problem to overcome the limitations of classical optimization techniques. A wide variety of heuristic optimization techniques have been applied such as genetic algorithm (GA) [2, 3], simulated annealing (SA) [4], Tabu search [5], and particle swarm optimization (PSO) [6]. The results reported in the literature were promising and encouraging for further research in this direction.

In 1995, Price and Storn [1] proposed a new floating point encoded evolutionary algorithm for global optimization and named it Differential Evolution owing to a special kind of differential operator, which they invoked to create new offspring from parent chromosomes instead of classical crossover or mutation. Easy methods of implementation and negligible parameter tuning made the algorithm quite popular very soon. The algorithm is inspired by biological and sociological motivations and can take care of optimality on rough, discontinuous and multi-modal surfaces. The DE has three main advantages: it can find near optimal solution regardless the initial parameter values, its convergence is fast and it uses few number of control parameters. In addition, DE is simple in coding, easy to use and it can handle integer and discrete optimization [7-10]. Differential evolution (DE) is a method that optimizes a problem by iteratively trying to improve a candidate solution with regard to a given measure of quality. Differential Evolution optimizes a problem by maintaining a population of candidate solutions and creating new candidate solutions by combining existing ones according to its simple formulae, and then keeping whichever candidate solution has the best score or fitness on the optimization problem at hand.

Originally Price and Storn [1] proposed a single strategy for differential evolution, which they later extended to ten different strategies. Differential evolution has been successfully applied to a wide range of problems including Batch Fermentation Process, Optimal design of heat exchanges, synthesis and optimization of heat integrated distillation system, etc. The performance of DE algorithm was compared to that of different heuristic techniques. It is found that, the convergence speed of DE is significantly better than that of GA [4, 5]. In the performance of DE was compared to PSO and evolutionary algorithms (EAs). The comparison was performed on a suite of 34 widely used benchmark problems. It was found that, DE is the best performing algorithm as it finds the lowest fitness value for most of the problems considered in that study. Also, DE is robust; it is able to reproduce the same results consistently over many trials, whereas the performance of PSO is far more dependent on the randomized initialization of the individuals [11]. In addition, the DE algorithm has been used to solve high-dimensional function optimization (up to 1000 dimensions) [12]. It is found that, it has superior performance on a set of widely used benchmark functions. Therefore

DE algorithm seems to be a promising approach for engineering optimization problems. It has successfully been applied and studied to many artificial and real optimization problems [13-17].

In this paper, a novel DE-based approach is proposed to solve the chemical process optimization problems and aimed at finding the global optimum solution for which the cost is to be optimized. The problem is formulated as a linear and non-linear optimization problem with equality and inequality constraints [18]. This study aimed at finding the global optimum solution for chemical processes for which cost is to be optimized. The optimization is carried out by evolutionary differential evolution algorithm. Additionally, the results are compared to those reported in the literature and with other conventional and non-conventional techniques.

II. DIFFERENTIAL EVOLUTION ALGORITHM

Optimization refers to finding one or more feasible solutions, which correspond to extreme values of one or more objectives. The need for finding such optimal solutions in a problem comes mostly from the extreme purpose of either designing a solution for minimum possible cost of fabrication, or for maximum possible reliability, or others [19, 20]. Because of such extreme properties of optimal solutions, optimization methods are of great importance in practice, particularly in engineering design, scientific experiments and business decision making.

In recent years, evolutionary algorithm have been applied to the solution of non-convex problem in many engineering application such as optimal design of an auto thermal ammonia synthesis reactor, which presents the effective use of DE to optimize the systems objective function subject to a number of equality constraints involving solution of coupled differential equations[21, 22]. Babu et al presented a case study on Optimization of thermal cracking operation, where optimization of thermal cracker carried out using DE [23]. DE exhibit difficulties in dealing with equality constraint problem but in general, they are the most efficient in terms of function evaluation. The differential evolution approach is presented for multi-objective optimization problems in optimization of adiabatic styrene reactor. The proposed algorithm is applied to determine the optimal operating condition for the manufacture of styrene [24]. In case of optimal design of gas transmission network, an evolutionary computation technique has been successfully applied for the optimal design of gas transmission network. The proposed strategy takes less computational time to converge when compared to the existing technique without compromising with the accuracy of the parameter estimates [14]. The first successful application of DE has been presented by Babu and Munawar for the optimal design of shell and tube heat exchanger [25] and optimization of an alkylation reaction to determine the optimal operating conditions for the alkylation process [26].

Differential evolution (DE) is a generic name for group of algorithms that are based on the principle of genetic algorithm (GA) but have some inherent advantages over genetic algorithm. Differential evolution algorithms are very robust and efficient in that they are able to find the global optimum of a function with ease and accuracy [19]. Differential evolution algorithms are faster than genetic algorithms. Genetic algorithm evaluates the fitness of a point to search for the optimum. In other words, genetic algorithms evaluate vectors suitability. In differential evaluation, this vectors suitability is called its cost or profit depending on whether the problem is a minimization or a maximization problem. In differential evolution, no coding is involved and floating-point numbers are directly used [20, 21].

Choice of DE key parameters: NP should be 5-10 times the value of D, that is, the dimension of the problem. Choose F=0.5 initially. If this leads to premature convergence, then increase F. The range of values of F is 0<F<1.2, but the optimal range is 0.4<F<1.0. Values of F<0.4 and F>1.0 are seldom effective. CR=0.9 is a good first guess. Try CR=0.9 first and then try CR=0.1. Judging by the speed, choose a value of CR between 0 and 1[1].

III. DE COMPUTATIONAL FLOW

The main features of the DE algorithm can be stated as follow and also represented in fig.1:

Step 1: Population initialization: Initialize population randomly between the given upper and lower bounds for all the parameters.
Step 2:Cost evaluations: calculate the objective function value for initial population.
Step 3:Mutation and crossover

Take i as population counter i = (0, 1, 2… 19)
Randomly choose 3 population points a, b, and c such that i≠a≠b≠c
Select randomly a parameter j for mutation (j=0, 1)
Generate a random number[0,1]
If random number < CR,
Trial [j] =x_1 *[c] [j] + F (*x_1 *[*a_1*] [j] -* x_1 *[b] [j])*
If random number > CR,
Trial [j] = x_1 *[i] [j]*
Check for bounds:
If bounds are violated, then randomly generate the parameter as shown below:
Trial [j] = lower limit + rand.no. [0, 1] (upper limit - lower limit);

Repeat 3 till all parameters are mutated.
Step 4:Evaluations: Calculate the objective function value for the vector obtained after mutation and crossover.
Step 5: Selection: Select the least cost vector for next generation, if the problem is of minimization.
Step 6: Repeat: Repeat step 3 to 5 for a specified number of generations, or till some termination criterion is met.

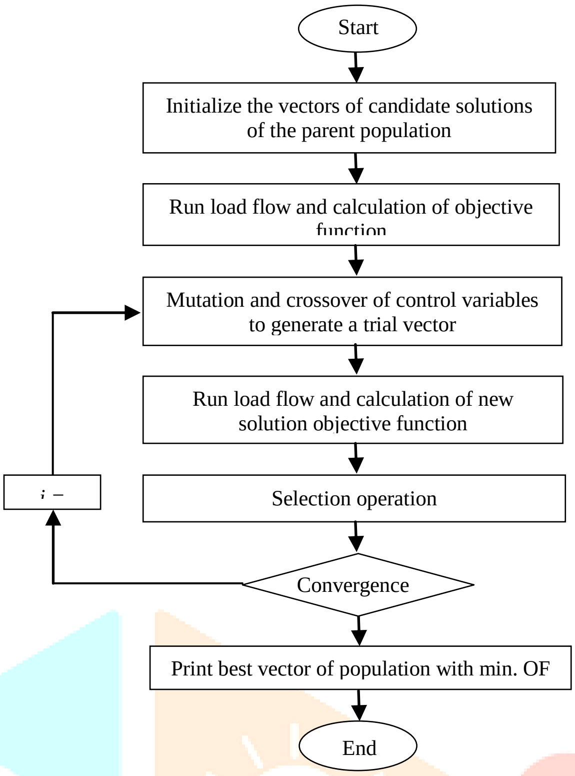

Figure 1: Flowchart for differential evolution algorithm

IV. CASE STUDIES

Problem Statement-1

The Objective function which is minimized using DE is given below

Minimize $f = (x_1{}^2 + x_2 - 11)^2 + (x_1 + x_2{}^2 - 7)^2$

Which subject to constraint $0 \le x_1$ and $x_2 \le 6$

Problem Statement-2

A chemical company produces two chemical products that produced through two different parallel reactions as shown below

$$A + B \xrightarrow{k1} P_1$$
$$A + B \xrightarrow{k2} P_2$$

The raw materials A and B have limited supply of 36 kg and 14 kg per day respectively. The reaction 6.11a takes 3 kg A and 1 kg B to produce 1 kgP_1, and the reaction 6.11b takes 2 kg A and 1 kg B to produce 1 kgP_2. The profit of the company from these products is \$14 per kg $P_1$and \$11 per kgP_2. Formulate a linear programming problem and maximize the daily profit of the company.

Maximize, $f = 14x_1 + 11x_2$

Subject to: $3x_1 + 2x_2 \le 36$

$x_1 + x_2 \le 14$

$x_1, x_2 \ge 0$

V. RESULTS AND DISCUSSION

The performance of differential evolution algorithm is tested by applying it to above problems. The key parameter of DE- Crossover Ratio (CR), Number of population size (NP), Scaling Factor (F), and Number of iterations are varied over a wide range of their possible values.

The above two optimization problems are solved by using differential evolution and conventional techniques and the results are obtained as shown in table 1 and table 2. The results obtained by differential evolution are compared with the conventional techniques; it is found that differential evolution is more suitable as compared to conventional techniques.

Implementation: The proposed DE algorithm is developed and implemented using the MATLAB software. Initially, several runs are done with different values of DE key parameters such as differentiation (or mutation) constant F, crossover constant CR, size of population NP, and maximum number of generations GEN which is used here as a stopping criteria. In this paper, the following values are selected as:

For problem statement 1: F = 0.8; CR = 0.5; NP = 20; GEN = 20
For problem statement 2: F = 0.8; CR = 0.9; NP = 20; GEN = 20

Problem statement 1 is minimization problem where answers by conventional methods are 3.1 for x_1, 2.01 for $x_2$and value of function is 0.404. Whereas by using DE the answers are 2.9 for x_1,2.03 for $x_2$and value of function is 0.314.Problem statement 2 is maximization problem where answers by conventional methods are 8 for x_1,6 for $x_2$and value of function is 178. By using DE the answers are 5.62 for x_1, 7.1 for $x_2$and value of function is 156.78.

Table 1:Solution for Problem Statement-1

GEN	x_1	x_2	*f(x)*	*GEN*	x_1	x_2	*f(x)*
Ind. 1	1.5	2.3	41.646	Ind. 11	1.46	3.23	55.7320
Ind. 2	1.98	2.8	26.267	Ind. 12	2.1	5.7	762.00
Ind. 3	2.26	3.0	26.514	Ind. 13	3.4	2.08	7.4973
Ind. 4	2.55	3.92	119.50	Ind. 14	0.52	3.33	75.996
Ind. 5	2.92	5.2	534.59	Ind. 15	1.09	3.9	121.44
Ind. 6	3.2	5.5	722.07	Ind. 16	2.9	2.03	0.314
Ind. 7	3.1	4.6	308.21	Ind. 17	1.46	4.1	22.738
Ind. 8	1.24	4.8	320.34	Ind. 18	4.8	1.9	196.31
Ind. 9	2.5	3.9	115.43	Ind. 19	2.5	4.5	248.12
Ind. 10	2.5	1.92	8.671	Ind. 20	2.8	3.4	54.22

Table 2:Solution for Problem Statement-2

GEN	x_1	x_2	*f(x)*	*GEN*	x_1	x_2	*f(x)*
Ind. 1	1	2.5	41.5	Ind. 11	3.5	5	104
Ind. 2	1.25	2.80	48.3	Ind. 12	3.82	5.39	112.77
Ind. 3	1.5	3	54	Ind. 13	4	5.5	116.5
Ind. 4	1.65	3.25	58.85	Ind. 14	4.37	5.59	122.67
Ind. 5	2	3.5	66.5	Ind. 15	4.5	6	129
Ind. 6	2.37	3.85	75.53	Ind. 16	3.9	5.4	114
Ind. 7	2.5	4	79	Ind. 17	4.228	6.5	133.492
Ind. 8	2.95	4.90	95.2	Ind. 18	4.4	6.92	137.72
Ind. 9	3	4.5	91.5	Ind. 19	4.658	7	142.212
Ind. 10	3.23	4.87	98.79	Ind. 20	5.62	7.1	156.78

VI. CONCLUSION

Differential Evolution optimization algorithm has been proposed, developed and successfully applied to solve chemical processes and simple mathematical problems. A generalised procedure has been developed to solve optimization problem by using Differential Evolution. Two chemical engineering case study problems have been solved using DE in the present work. The evolutionary algorithm gives a list of good choice of parameters which helps to achieve better result with less effort. Results indicate that DE is more reliable, efficient and hence a better approach to the optimization of non-linear problems.

Due to simple structure, ease of use, speed and robustness, it has been shown that Differential Evolution is the more appropriate choice for optimization. Differential Evolution technique is much faster, has less computational burden when compared to non-traditional techniques and the estimation is much more accurate and efficient. The search for the global minimum is strongly dependent on the control parameters. Differential evolution requires less number of function evaluations and assures convergence from any starting point. Differential evolution has been proved to be really efficient when solving chemical process problems. Hence differential evolution is a potential tool for accurate and faster optimization. On the basis of results of above solved problems we conclude that differential evolution explores the decision space more efficiently than conventional and non-conventional techniques. Differential Evolution is more effective in obtaining better quality solutions.

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