Differential Evolution (DE) Algorithm: Population Based Metaheuristic Search Algorithm for Optimization of Chemical Processes

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Abstract: *Differential Evolution (DE) is an evolutionary optimization technique that is very simple, fast, and robust at numerical optimization. It has mainly three advantages; finding the true global minimum regardless of the initial parameter values, fast convergence, and using few control parameters. The main advantage of the DE over other methods is its stability. DE algorithm is a population based algorithm like genetic algorithms using similar operators; crossover, mutation and selection. DE 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 two chemical engineering problems from the literature. The comparison is made with some other well-known conventional and non-conventional optimization methods. From the 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 [1]. 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 [2, 8-12]. 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 problems to overcome the limitations of classical optimization techniques. A wide variety of heuristic optimization techniques have been applied such as genetic algorithm (GA) [3, 4], simulated annealing (SA) [5], Tabu search [6], and particle swarm optimization (PSO) [7]. The results reported in the literature were promising and encouraging for further research in this direction.

In 1995, Price and Storn [2] proposed a new evolutionary algorithm for global optimization and named it DE 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 of the initial parameter values, its convergence is fast and it uses a few number of control parameters. In addition, DE is simple in coding, easy to use and it can handle integer and discrete optimization [8-11].

DE is a method that optimizes a problem by iteratively trying to improve a candidate solution with regard to a given measure of quality. DE 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 [2] proposed a single strategy for DE, which they later extended to ten different strategies. DE has been successfully applied to a wide range of problems including Batch Fermentation Process, Optimal design of heat exchangers, synthesis and optimization of heat integrated distillation system, etc. The performance of the 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 [5, 6]. 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. In addition, 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 [12]. In addition, the DE algorithm has been used to solve high-dimensional function optimization (up to 1000 dimensions) [13]. It is found that it has superior performance on a set of widely used benchmark functions. Therefore, the 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 [14-18].

Keller et al [19] applied DE algorithm to find the minimum total annualized cost of the non-equilibrium reactive distillation for the synthesis of ethylene glycol, which is a MINLP optimization problem. This paper result shows that the optimized objective function values are better than those reported literature value and DE strategy (DE/best/1/bin) is a capable of providing optimized solutions which are close to the global optimum and reveals it’s adequacy for the optimization of reactive distillation problems encountered in chemical engineering practice. Kai Yit Kok and Rajendran P. [20] have widely applied the DE algorithm on unmanned aerial vehicle (UAV) path planning. Instead of using trial and error, this paper presents an optimization method of DE algorithm for tuning the parameters of UAV path planning. The proposed optimization of tuning parameters in DE algorithm for UAV path planning expedites and improves the final output path and computational cost. Das et al [21] explored several schemes for controlling the convergence behaviors of particle swarm optimization and DE by judicious selection of their parameter. This article discussed the mutual synergy of particle swarm optimization with DE leading to a more powerful global search algorithm and its practical application [22].

In this paper, two chemical process optimization problems were selected to find 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. The optimization is carried out by an evolutionary DE algorithm. Additionally, the results are compared to those reported in the literature and with other conventional and non-conventional techniques..

II. DIFFERENTIAL EVOLUTIONARY 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 [23, 24]. 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[25, 26]. Babu et al presented a case study on Optimization of thermal cracking operation, where optimization of thermal crackers was carried out using DE [27]. DE exhibits difficulties in dealing with equality constraint problems but in general, they are the most efficient in terms of function evaluation. The DE approach is presented for multi-objective optimization problems in optimization of adiabatic styrene reactors. The proposed algorithm is applied to determine the optimal operating condition for the manufacture of styrene [28]. In the 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 [15]. The first successful application of DE has been presented by Babu and Munawar for the optimal design of shell and tube heat exchanger [29] and optimization of an alkylation reaction to determine the optimal operating conditions for the alkylation process [30].

DE is a generic name for a group of algorithms that are based on the principle of Genetic Algorithm (GA) but have some inherent advantages over genetic algorithms. DE algorithms are very robust and efficient in that they are able to find the global optimum of a function with ease and accuracy [23]. DE 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 DE, this vector's suitability is called its cost or profit depending on whether the problem is a minimization or a maximization problem. In DE, no coding is involved and floating-point numbers are directly used [24, 25].

III. DE COMPUTATIONAL FLOW

The main features of the DE algorithm can be stated as follows and is represented in fig. 1 [31].

1- Population initialization: Initialize population randomly between the given upper and lower bounds for all the parameters.

2- Cost Evaluation: calculate the objective function value for initial population.

Step 3- Mutation and Crossover:
Take i as population counter i = (0, 1, 2… 19)

a. *Randomly choose 3 population points a, b, and c such that $i \neq a \neq b \neq c$*
b. *Select randomly a parameter j for mutation (j=0, 1)*
c. *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 until all parameters are mutated.

4- Evaluation: Calculate the objective function value for the vector obtained after mutation and crossover.

5- Selection: Select the least cost vector for the next generation, if the problem is of minimization.

6- Repeat: Repeat step 3 to 5 for a specified number of generations, or till some termination criterion is met.

IV. PRESENT WORK

4.1 Objective

The objective of the present work was aimed at finding the global optimum solution for chemical processes for which cost is to be optimized. The optimization is carried out by an evolutionary DE algorithm and the results obtained are compared with other conventional and non-conventional techniques. The analytical solution of the DE optimization problem involves a number of iterations and they are time consuming. Hence, a MATLAB code is generated for each problem under consideration to arrive at an optimal solution.

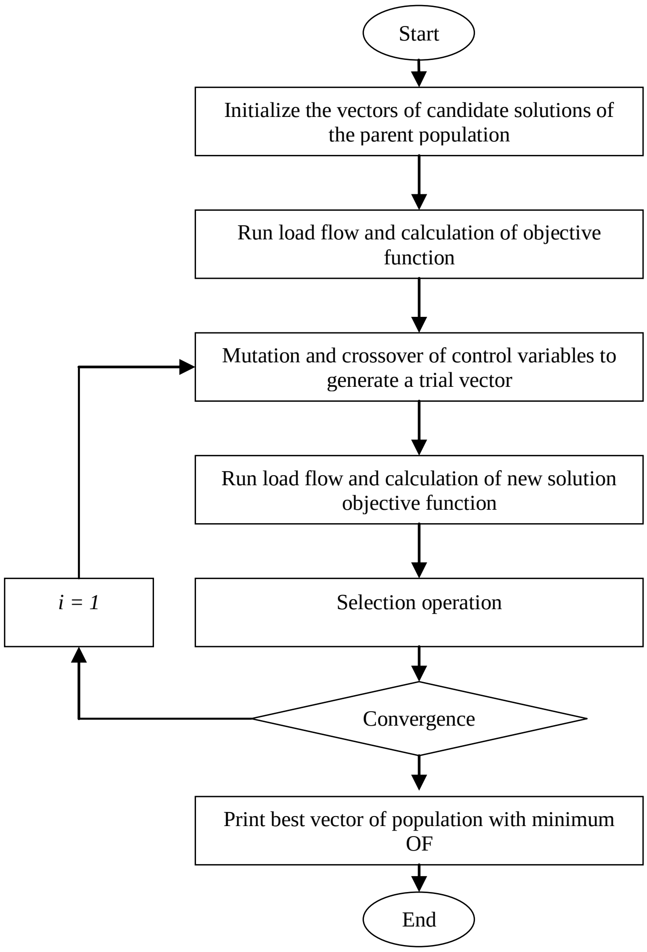

Figure 1: Flowchart for DE Algorithm

4.2 Problem: 1

Optimization of Biological Wastewater Treatment Plant

A rectangular tank has been made for biological treatment of wastewater (batch process). The dimensions of the tank are given in Fig.2 (Length x^1 meters, width x^2 meters, and height x^3 meters). The sides and bottom of the tank cost, respectively, Rs. 1200/-, and Rs. 2500/- per m^2 area. The operating cost for the tank is Rs. 500/- for each batch of water treatment. Maintenance cost of Rs. 100/- for every 10 batches is required. Assuming that the tank will have no salvage value, find the minimum cost for treatment of 1000 m^3 of wastewater. Assume the salvage value of the tank is zero after 1000 m^3 of wastewater treatment [32].

4.3 Problem: 2

Optimization of liquid storage tank

A cylindrical tank shown in Fig. 3 has a volume (*V*) that can be expressed by $V = (\pi/4)\, D^2 L$, and we are interested in calculating the diameter (*D*) and height (*H*) that minimize the cost of the tank [32].
Cost of the tank is given by f; we will get the optimum design by solving the nonlinear problem:

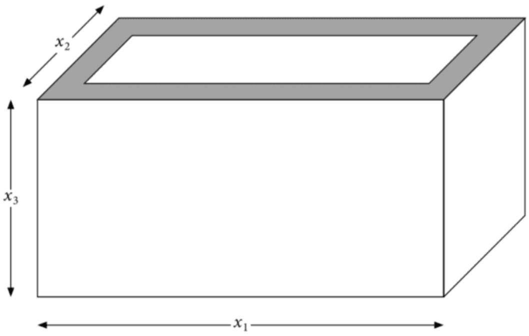

Figure 2: Biological wastewater treatment plant

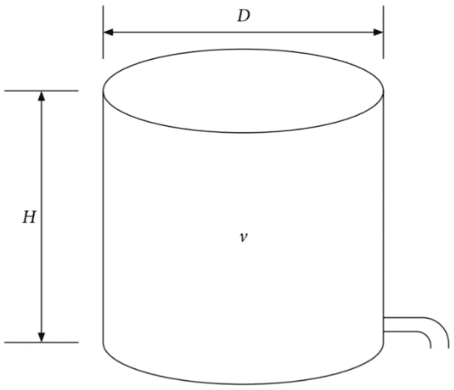

Figure 3: Liquid storage tank

$$\min_{H,D} f = C_s \pi DH + C_t (\pi/2)D^2$$

Subject to, $V = (\pi/4)D^2 H$, $D \geq 0$, $H \geq 0$

The cost of the tank depends on the amount of material needed which is proportional to its surface area and the cost per unit area of the tank's side is C_s, whereas for tank's top and bottoms the cost per unit area is C_t .

We are able to simplify the problem by ignoring the bound constraints and eliminating the variable H from the above Equation, giving us an unconstrained problem:

$$f = 4C_s V/D + C_t(\pi/2)D^2$$

Now, applying necessary condition for minimization; the objective function is differentiated with respect to D and setting the derivative to zero yields

$$\frac{df}{dD} = -4C_s V/D^2 + C_t \pi D = 0\,,$$

Which yielding, $D = \left(\frac{4C_s V}{\pi C_t}\right)^{1/3}$, $H = \left(\frac{4V}{\pi}\right)^{1/3}\left(\frac{C_t}{C_s}\right)^{2/3}$ and the aspect ratio. $H/D = C_t/C_s$

V. RESULT AND DISCUSSIONS

The performance of the DE algorithm is tested by applying it to above problems. The key parameters 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 DE and conventional techniques and the results are obtained as shown in Table 1 and Table 2. The results obtained by DE are compared with the conventional techniques; it is found that DE is more suitable as compared to conventional techniques.

Implementation:

The proposed DE algorithm is developed and implemented using the MATLAB software. Initially, several runs were 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* = 30; *GEN* = 30

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

Table 1: Solution for Problem Statement-1

GEN	x^1	x^2	x^3	*f(x)*
Ind. 1	1	4.2	1	144.41
Ind. 2	5	4.4	10	283.03
Ind. 3	7.29	5	5	287
Ind. 4	6.24	6	5	258.18
Ind. 5	3.136	3	5.84	118.8
Ind. 6	4	5	4.522	153.31
Ind. 7	3.4	2.8	3.2	88.16
Ind. 8	4.89	5.02	2.59	131
Ind. 9	2.56	1.124	3.25	90.69
Ind. 10	3.848	2.9	5.68	126.94
Ind. 11	7.56	4.67	3.872	205.55
Ind. 12	4.57	5.87	4.44	185.22
Ind. 13	6.5	2.8	3.1	123.73
Ind. 14	1	3.5	5.7	95.87
Ind. 15	4.7	3.8	7.8	207.43
Ind. 16	5.42	1.3	3.4	93.75
Ind. 17	5.7	2.64	4.56	188.31
Ind. 18	2.9	3.2	4.7	103.7
Ind. 19	1.8	2.5	3.5	79.75
Ind. 20	6.3	2.9	2.1	105.34
Ind. 21	2.3	8.5	3.8	154.24
Ind. 22	3.9	2.4	5.2	112.5
Ind. 23	2	1.78	3.9	81.01
Ind. 24	3.2	6.4	3.8	145.3
Ind. 25	4.8	6.54	2.9	14248.1
Ind. 26	1.66	7.3	3.8	122.82
Ind. 27	5.4	3.12	2.9	111.86
Ind. 28	3.2	2.5	3.9	40938.7
Ind. 29	4.9	2.56	3.8	110.09
Ind. 30	4.5	2.7	3.62	104.52

Solution for problem 1:

The total cost of water treatment = Cost of the tank + operating cost of wastewater treatment + maintenance cost = (cost of side + cost of bottom) + number of batch × (cost for each batch) + 100 × (number of batch)/10

$$f(x) = 1200(2x_1x_3 + 2x_2x_3) + 2500x_1x_2 + 500\left(\frac{1000}{x_1x_2x_3}\right) + 100\left(\frac{100}{10x_1x_2x_3}\right)$$

$$x_1x_2x_3 \leq 10$$

The value represented here is $f(x) = \frac{F(x)}{1000}$

Problem statement 1 is a minimization problem where the answers by using DE (refer Table 1) are 1.8 m for length x_1, 2.5 m for width x_2, 3.5 m for height x_3 and the minimum value of the cost of water treatment is Rs. 79750/-.

Table 1: Solution for Problem Statement-2

GEN	*D*	*H*	*f(x)*
Ind. 1	5	12	65777.09
Ind. 2	5.7	13.9	86468.8
Ind. 3	6.7	14.81	111426.4
Ind. 4	6.3	15.62	106901.72
Ind. 5	5.16	16.82	88031.76
Ind. 6	6.66	17.1	122621.4
Ind. 7	8.22	17.92	166105.73
Ind. 8	8.7	17.98	179331.14
Ind. 9	7.19	18.2	141347.55
Ind. 10	5.8	18.5	109372.98
Ind. 11	6.5	19.23	129694.76
Ind. 12	5.9	19.75	117491.25
Ind. 13	7.3	19.92	153970.63
Ind. 14	7.27	19.67	151747.69
Ind. 15	6.896	18.435	135327.9
Ind. 16	7.636	18.694	161616.45
Ind. 17	6.956	20.638	1488521.3
Ind. 18	7.78	20.24	168836.4
Ind. 19	8.014	20.23	175250.77
Ind. 20	9.264	24.58	242876.32

Solution for problem 2:

In this problem, we considered the cost per unit area of the tank's side C_s is Rs. 250/- and tank's top and bottom cost per unit area C_t is Rs. 475/-. By using C_s and C_t values and applying DE method, (refer Table 2) we get diameter (*D*) as 5 meter, height (*H*) as 12 meter and minimum cost of the tank is Rs. 65777.09/-.

VI. CONCLUSIONS

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 problems by using DE. 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 results with less effort. Results indicate that DE is more reliable, efficient and hence a better approach to the optimization of non-linear problems.

DE has been proved to be really efficient when solving chemical process problems. Hence, DE is a potential tool for accurate and faster optimization. On the basis of case studies results, we conclude that DE explores is more efficient than conventional and non-conventional techniques. DE is more effective in obtaining optimal solutions.

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