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Computation of the Optimal Value of Operating Parameters in a Reactor – Heat Exchanger System by Differential Evolution Techniques

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Abstract: ***In this research work, the modern soft computing technique of Differential Evolution (DE) algorithm is considered to determine global optimal values of the operating parameters in a Reactor -Heat Exchanger (RHE) system. In addition, a penalty term is incorporated in the objective function and thereby computing annual cost of the RHE system in terms of operating and investment costs. A comparative study is also made with Genetic Algorithm (GA) in RHE system. Results clearly indicate the supremacy of DE for global optimization of operating parameters in RHE system. A convergence test is performed and reported here.***

Index Terms: Optimization, Differential Evolution Algorithm, Genetic Algorithm, Reactor - Heat Exchanger System.

I. INTRODUCTION

Problems which involve global optimization over continuous spaces [1] are everywhere throughout the scientific community. In general, the task is to optimize certain properties of the system by suitably choosing the system parameters. The optimal design of process plant is complex and involves several equality and inequality constraints. The advance of the computational resources has encouraged the utilization of optimization techniques in the solution of complex engineering problems. Thus, it is very attractive to consider the possibility of joining the feature of natural optimization methods to one algorithm which allows to work with small populations and to reduce computational time greatly. The standard approach to an optimization problem begins by designing an objective function which can model the problem's objectives while incorporating any constraints. The ability to handle non-differentiable, nonlinear and multimodal cost functions, parallelizability to cope with computation intensive cost functions and few control variables to steer the minimization are the salient futures of DE [2-4]. In general, the objective function, generally called as cost function seems to be nonlinear in nature [6-9]. The main contribution of this work involves the implementation of DE at Reactor - Heat Exchanger (RHE) System [5] to optimize the process variables and thereby minimize the annual cost. Here a penalty term is included in the objective function.

The organization of this paper is as follows. In section 2, description of the Differential Evolution (DE) in terns of Initialization, Mutation, Crossover, Evaluation-selection and Control parameter are presented. Mathematical model of Reactor - Heat Exchanger System is given in section 3. Results and Discussion is analyzed in section 4. Finally in section 5, a summing up of the entire work is given.

II. DIFFERENTIAL EVOLUTION

DE is a global optimization technique that is exceptionally simple, significantly faster and robust. The overall structure of the DE algorithm resembles that of most other evolutionary computation techniques i.e., population based search as shown in fig.2.1. The fittest of an offspring competes one-to-one with that of corresponding parent, which is different from the other evolutionary algorithms. This one-to-one competition gives rise to faster convergence rate. DE is the real coded genetic algorithm combined with an adaptive random search using a normal random generator. DE uses floating point numbers that are more appropriate than integers for representing points in a continuous space.

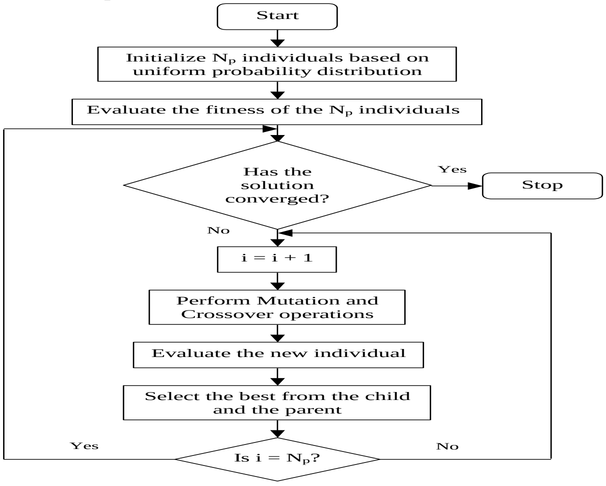

Fig.2.1. Flow chart of Differential Evolution Technique

A. *Initialization*

The initial population of N_P individuals is randomly selected based on uniform probability distribution for all variables to cover the entire search space uniformly. The initial population is represented as

$$Z_i^0 = Z_i^{min} + \rho\left(Z_i^{max} - Z_i^{min}\right)$$
$$i = 1\ldots N_P \text{ and } \rho \in [0,1] \qquad (1)$$

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B. *Mutation*

Differential evolution generates new parameter vectors by adding the weighted difference vector between two population members to a third member. The essential ingredient of mutation operation is the difference vector. A perturbed individual is therefore generated on the basis of the parent individual in the mutation process by

$$\hat{Z}_i^{G+1} = Z_p^G + F \times \left(Z_j^G - Z_k^G \right) \qquad F \in [0,1] \qquad (2)$$

The scaling factor F ensures the fastest possible convergence. The perturbed individual is essentially a noisy random vector of Z_p^G. The parent individual depends on the circumstance in which the type of the mutation operation is employed. If the new decision variable is out of the limits (lower and upper) by an amount, then, this amount is subtracted or added to the limit violated, to shift the value inside the limits.

C. *Crossover*

In order to extend the diversity of the new individuals in the next generation, the perturbed individual $\hat{Z}_i^{G+1}$ and the current individual Z_i^G are selected by a binomial distribution to perform the crossover operation to generate the offspring. In this crossover operation the gene of an individual at the next generation is produced from the perturbed individual and the present individual.

i.e.

$$\hat{Z}_i^{G+1} = \begin{cases} Z_{ji}^G, & \text{if a random number} > C_R \\ \hat{Z}_{ji}^{G+1}, & \text{otherwise} \end{cases}$$

$$i = 1 \ldots N_P,\ j = 1 \ldots n \qquad (3)$$

where the crossover factor $C_R \in [0,1]$ is assigned by the user.

D. *Evaluation and Selection*

In the evaluation process, an offspring competes one-to-one with the parent. The parent is replaced by its offspring if the fitness of the offspring is better than that of its parent. Defiantly the parent is retained in next generation if the fitness of offspring is worse than the parent. The first step involved in the evaluation process is one-to-one competition and the second step is the selection of best individual in the population as given by

$$Z_i^{G+1} = \arg\min \left\{ \psi\left(Z_i^G\right), \psi\left(\hat{Z}_i^{G+1}\right) \right\} \quad i = 1 \ldots N_P \qquad (4)$$

$$\hat{Z}_b^{G+1} = \arg\min \left\{ \psi\left(Z_i^{G+1}\right), i = 1, \ldots N_P \right\} \qquad (5)$$

Then the vector with lesser cost replaces the initial population. With the members of the next generation thus selected, the cycle repeats until the maximum number of generations or no improvement is seen in the best individual.

The minimization method in DE is self-organizing so that very little input is required from the user. DE's self-organizing scheme takes the difference vector of two randomly chosen population vectors to perturb an existing vector. The perturbation is done for every population vector. Therefore, DE is easy to use and requires only few control variables to steer the optimization. These variables are also robust and easy to choose. DE has good convergence properties that are mandatory for a good minimization algorithm. It consistently converges to the global minimum in consecutive independent trials.

E. *Differential Evolution Control Parameters*

Differential evolution presents great convergence characteristics and requires few control parameters, which remain fixed throughout the optimization process and need minimum tuning. The control parameters are the population size N_P, weight applied to the random differential F and crossover constant C_R. The selection of the control variables i.e., N_P, F and C_R is seldom difficult and some general guidelines can be followed. A reasonable choice for the population size is between 5 to 10 times the number of variables and N_P must be at least 4 to ensure that DE will have enough mutually different vectors with which to work. A value of F equal to 0.5 is usually a good initial choice. If the population converges prematurely, then F and/or N_P should be increased. The choice for C_R is 0.9 or 1.0 is appropriate in order to see if a quick solution is possible since a large C_R often speeds convergence.

III. PROBLEM FORMULATION

A. *Reactor and Heat Exchanger System*

The RHE system is shown in Fig.3.1. Here a first order exothermic reaction A→ B is considered. The goal in design of this system is to find the optimal design parameters such as reactor volume V, area of heat exchanger A and the flow rates F_1 & F_W, to energetic a minimum of 90% conversion of reactant. The constraint equations are formulated by making an independent rector material balance, energy balance, heat exchanger design and energy balances.

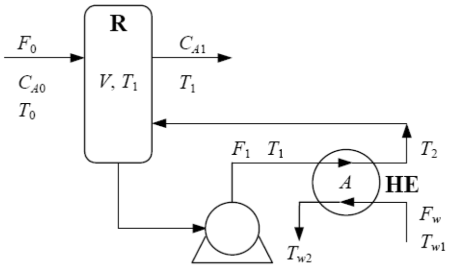

Fig.3.1. Reactor a Heat Exchanger System

B. *Design Objective*

The design objective of RHE system is to minimize the total plant cost ($/year) including the investment and operating costs in terms of volume, area and flow rates involved in the system and is given by

Total Annual

$$Cost = 691.2V^{0.7} + 873.6A^{0.6} + 1.76F_W + 7.056F_1 \qquad (6)$$

The first two terms of right side represents the investment cost and the other two terms is the operating cost involved in the system. The objective function is subject to equality and inequality constraints formed from the material and energy balance equations of the process. The constant parameter values for RHE system are given in Table3.1.

Table3.1. Parameter Values –RHE System

Parameters	Values
Concentration of A in the feed stream C_{A_0}	32.04 kmol/m³
Feed flow rate F_0	45.36 kmol/h
Feed Temperature T_0	333 K
Cooling water inlet temperature T_{w_1}	293 K
Arrhenius rate constant k_R	12 h⁻¹
Overall heat transfer coefficient U	1635 kJ/(m².h.K)
Ratio of activation energy to perfect gas constant E/R	555.6 K
Molar heat of Reaction $(-\Delta H_R)$	23260 kJ/kmol
Reactant heat capacity c_p	167.4 kJ/(kg.K)
Cooling water heat capacity c_{p_w}	4.184 kJ/(kg.K)

Reactor Material Balance

$$F_0 x_A - k_R \exp\left(-\left(E/RT_1\right)\right) C_{A_0}\left(1 - x_A\right)V = 0 \tag{7}$$

Reactor Heat Balance

$$F_0 C_P\left(T_0 - T_1\right) - F_1 C_P\left(T_1 - T_2\right) + \left(-\Delta H_R\right)F_0 x_A = 0 \tag{8}$$

Heat Exchanger Design Balance

$$F_1 C_P\left(T_1 - T_2\right) = Au\Delta T_{lm} \tag{9}$$

The logarithmic mean temperature $\left(\Delta T_{lm}\right)$ is given by

$$\left(\Delta T_{lm}\right) = \frac{\left(T_1 - T_{w2}\right) - \left(T_2 - T_{w2}\right)}{\ln\dfrac{\left(T_1 - T_{w2}\right)}{\left(T_2 - T_{w2}\right)}} \tag{10}$$

Heat Exchanger Energy Balance

$$F_1 C_P\left(T_1 - T_2\right) = F_w C_{P_w}\left(T_{w_2} - T_{w_1}\right) \tag{11}$$

Temperature Bounds

$$311 \le T_1 \le 389K\ ,\ 311 \le T_2 \le 389K \text{ and}$$

$$300 \le T_{w_2} \le 380K \tag{12}$$

Heat Exchanger Operation Constraints

$$T_1 - T_2 \ge 0\, , T_{w_2} - T_{w_1} \ge 0\ T_1 - T_{w_2} \ge 11.1 \text{ and}$$

$$T_2 - T_{w_1} \ge 11.1 \tag{13}$$

Quality Constraint

$$x_A \ge 0.90 \tag{14}$$

C. *Solution Methodology*

A penalty function approach is used to handle the explicit constraints. Penalty terms are incorporated in the objective function, which reduce the fitness of the string according to the magnitude of their violations. The modified objective function for the design of RHE system is given as

$$\psi = 691.2V^{0.7} + 873.6A^{0.6} + 1.76F_w + 7.056F_1 + \lambda\left[\sum_{z \in LVC}^{N}\left|C_z - C_{z(\text{limit})}\right|\right] \tag{15}$$

IV. RESULTS AND DISCUSSION

The computational works are carried out in the platform of C++ in Core (TM) Due 1.66 GHz processor. The results obtained using DE for the design optimization of RHE system are recorded and presented in fig.4.1 to fig.4.5.

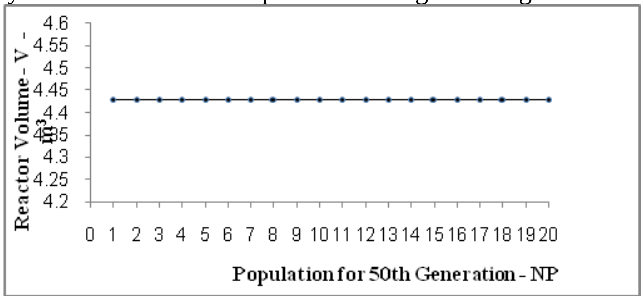

Fig4. 1. Population Vs Reactor Volume – at 50th Generation

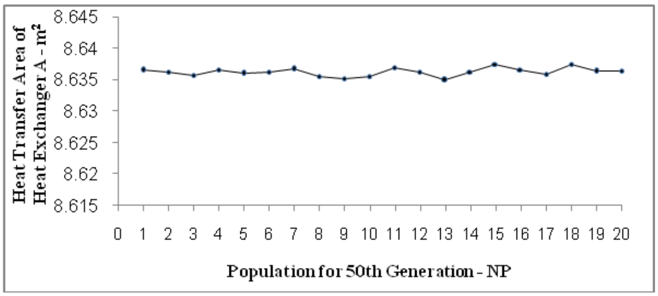

Fig.4. 2. Population Vs Heat Transfer Area – at 50th Generation

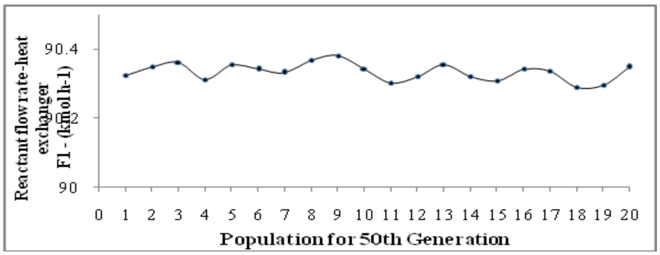

Fig.4. 3. Population Vs Reactant Flow Rate – at 50th Generation

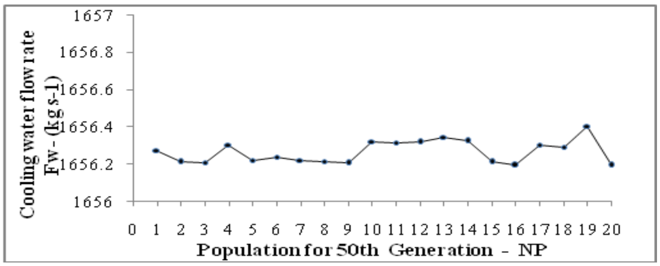

Fig. 4. 4. Population Vs Cooling Water Flow Rate – at 50th Generation

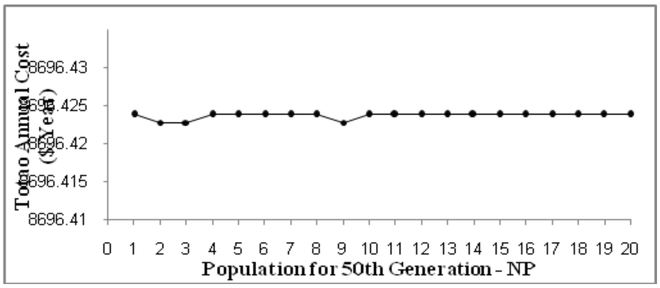

Fig.4. 5. Population Vs Total Annual Cost – at 50th Generation

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A comparison of this result with the design results of GA is reported in table 4.1.

Table4.1 Performance analysis of DE based optimal design with GA in RHE System

Variables	GA	DE
V (m3)	4.893	4.423
A(m2)	7.453	8.636
T1(K)	389	389
T2 (K)	353.5	354.33
Tw2 (K)	355.0	368.666
Fw(103 kg/h)	2.279	1.656
F1 (kg mol/h)	88.32	90.347
Investment Cost ($/year)	5015.91	5143.423
Operating Cost ($/year)	4634.23	3552.467
Total Annual Cost ($/year)	9650.14	8696.423
CPU Time (s)	3	0.061

It is observed that the proposed approach lands at the optimum value (Total Annual Cost ($ 8696.423). The CPU time is also found to be much smaller than others. (0.061s).

In addition, evolutionary computation control parameters employed in this works are furnished in Table4.2 and the convergence of the global optimal using DE is presented in fig.4.6.

Table4.2. Control Parameters

Control Parameters	Symbol	Value
Population for each Generation	NP	20
Weight Applied to Random Differential	F	0.75
Crossover Constant	C_R	1.0

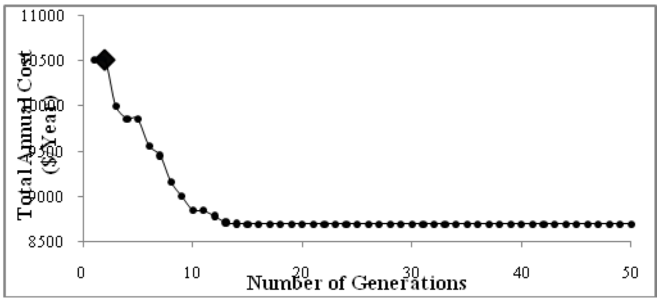

Fig.4. 6. Convergence of Global Optimal using DE

The present approach of finding design variables using DE is benefited from the fact that it never employs complicated mathematical computations and procedures as the algorithm is simple in nature and also found to be proficient in solving the complex problem with several variables and nonlinear constraints.

V. CONCLUSION

This paper demonstrates the successful implementation of Differential Evolution technique in the optimal design of RHE system. The result clearly indicates that DE is found to be better technique than Genetic Algorithm in optimal design of RHE system. Faster convergence rate, Simple mathematical formulation of problem, Efficient handling of problems with large number of discrete variables and constraints are the salient features of DE. Due to its simplicity and ease in implementation in optimal design of RHE system, this DE computing techniques is proved to be an efficient and effective alternative for Genetic Algorithm.

REFERENCES

1. Storn.R., Price.K,, Differential Evolution – A simple and efficient adaptive scheme for global optimization over continuous spaces, Technical Report TR-95-012, International Computer Science Institute, Berkeley, 1995.
2. Storn.R.,Price.K., Differential Evolution – A Simple and Efficient Heuristic for Global optimization over Continuous Spaces, Journal of Global Optimization,Vol.11**,** 1997. pp.341 – 359.
3. Price K., Storn R., Lampinen J., Differential Evolution - A Practical Approach to Global Optimization, Springer, Berlin, 2005.
4. Millie Pant, Radha Thangaraj and V. P. Singh, Optimization of Mechanical Design Problems Using Improved Differential Evolution Algorithm, International Journal of Recent Trends in Engineering, Vol. 1, No. 5, 2009,pp.21 -25.
5. Fernando P. Bernardo., Efstratios N. Pistikopoulos .,Pedro M. Saraiva .,Quality costs and robustness criteria in chemical process design optimization,Computer and Chemical Engineering Journal,Vol.25,2001,pp.27 – 40.
6. Fernando P. Bernardo., Pedro M. Saraiva .,Robust optimization framework fo process parameter and tolerance design. AICHE Journal, Vol. 44(9), 1998, pp.2007–2017.
7. Halemane.K.P., Grossmann.I.E., Optimal process design under uncertainty. AICHE Journal,Vol. 29(3),1983,pp.425–433.
8. Vikrant Bansal,John D. Perkins,and Efstratios N. Pistikopoulos ., Flexibility analysis and design using a parametric programming framework. AICHE Journal, Vol.48(12),2002,pp.2851–2865.
9. Grossmann.I.E., David A. Straub. Recent developments in the evaluation and optimization of flexible chemical processes. In COPE91, pp. 41. Elsevier, 1991.
10. Gopalakrishnan.B , Govindarajan.L ,Karunanithi.T and Bhaba.P.K , Genetic Algorithm Based Design Optimization Of Reactor - Heat Exchanger System , Modeling and Simulation, Allied Publisher ,Vol. 1,2007,pp. 214 – 219.

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