# Uncertainty of Operating Parameters in a Reactor – Heat Exchanger System

B.Gopalakrishnan[1], S.Raja[1], P.K.Bhaba

[1]Assistant Professor, Department of Chemical Engineering, Annamalai University, Annamalai Nagar, India - 608002

---***---

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. The uncertainty associated with a piece of knowledge provides a measure of its practical robustness. The targeted sample data for the control variables are collected from the stimulated DE to measure the level of uncertainty. Identify the sample data are within are out of control by using $\bar{X}$ and S control charts.

Key Words — Optimization, Differential Evolution Algorithm, Genetic Algorithm, Reactor - Heat Exchanger System, uncertainty.

## 1. 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 uncertainty associated with a piece of scientific knowledge provides a measure of its practical epistemological robustness. It represents the degree to which our knowledge concerning the relevant physical phenomenon is imperfect. Although uncertainty may be minimized, it cannot be eliminated: it is inherent to all scientific knowledge. Fortunately, science has developed methods for rigorously characterizing and communicating the level of uncertainty associated with certain types of claims.

The X bar and S control chart, shows the sample data drawn from the stimulated DE are within the upper and lower control limit.The organization of this paper is as follows. In section 2, description of the Differential Evolution (DE) in terms of Initialization, Mutation, Crossover, Evaluation-selection , Control parameter and control variables limits using X bar and S chart 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.

## 2. 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.

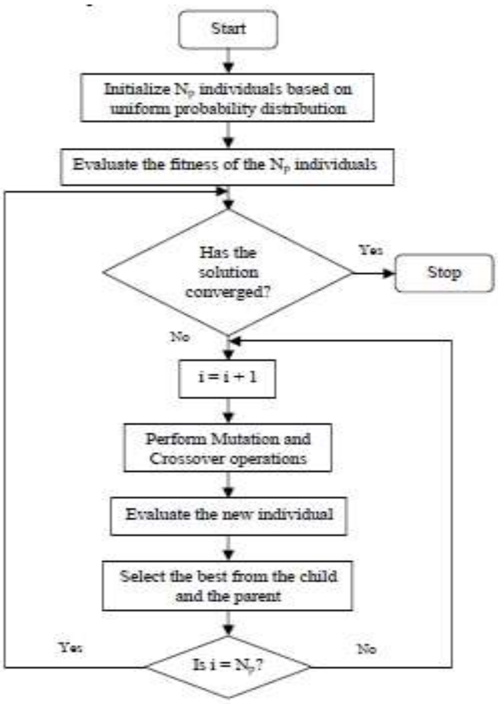



Fig.2.1. Flow chart of Differential Evolution Technique

Initialization

The starting populace of NP people is arbitrarily chosen taking into account uniform likelihood circulation for all variables to cover the whole hunt space consistently. The beginning populace is spoken to as

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

Mutation

Differential evolution creates new parameter vectors by including the weighted distinction vector between two populace individuals to a third part. The fundamental element of mutation operation is the distinction vector. An annoyed individual is accordingly produced on the premise of the guardian singular in the mutation handle by

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

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 relies on upon the situation in which the sort of the mutation operation is utilized. On the off chance that the new choice variable is out of the cutoff points (lower and upper) by a sum, this sum is subtracted or added as far as possible damaged to move the worth inside the breaking points.

Crossover

Keeping in mind the end goal to broaden the differing qualities of the individuals in the cutting edge, the perturbed individual and the present individual are chosen by a binomial dissemination to perform the crossover operation to create the posterity. In this crossover operation the quality of a person at the cutting edge is created from the perturbed individual and the present person.

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

$i = 1 \ldots N_P$, $j = 1 \ldots n$ where the crossover factor $C_R \in [0,1]$ is assigned by the user.

Evaluation and Selection

In the assessment prepare a posterity contends balanced with the guardian. The guardian is supplanted by its posterity if the fitness of the posterity is superior to anything that of its guardian. Conversely the guardian is held in cutting edge if the fitness of posterity is more terrible than the guardian. The primary step included in the assessment procedure is coordinated rivalry and the second step is the determination of best individual in the populace as given by

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

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

At that point the vector with lesser expense replaces the beginning populace. With the individuals from the cutting edge in this way chose, the cycle rehashes until the greatest number of eras or no change is found in the best person. Figure 2.1 demonstrates the strides included in fundamental differential evolution.

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 NP, weight applied to the random differential F and crossover constant CR. The selection of the control variables i.e., NP, F and CR 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 NP 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 NP should be increased. The choice for CR is 0.9 or 1.0 is appropriate in order to see if a quick solution is possible since a large CR often speeds convergence.

X-Bar and S Chart for Variables Data

The X-Bar (arithmetic) mean is used with variables data when sample size is between 2 and 30. The steps for constructing this type of Control Chart are

STEP1 - Determine the data to be collected.

STEP 2 - Collect the set of operating parameter data by subgroup which drawn the sample from stimulate DE. A subgroup is made up of variables data that represent a characteristic of a parameter by a process. Enter the individual subgroup measurements in time sequence in the portion of the data collection section of the Control Chart

STEP 3 – Calculate and enter the average for each subgroup. Use the formula below to calculate the average (mean) for each subgroup and enter it on the line labeled Average in the data collection section

$$\bar{X} = \frac{X_1 + X_2 + X_3 \ldots\ldots\ldots\ldots X_n}{n}$$

Where $\bar{X}$ is Average of the within each subgroups $X_1, X_2, X_3 \ldots\ldots\ldots X_n$ is the individual observation within a subgroup n is total number observation within a subgroup

Step 4 – Calculate and enter the standard deviation ($\sigma$) for each subgroup. Use the following formula to calculate the standard deviation ($\sigma$) for each subgroup. Calculate the standard deviation value using the formula given below

$$\text{Sigma } (\sigma) = \text{standard deviation} = \sqrt{\frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{n-1}}$$

Where $X_i$ is individual observed value.

STEP 5 - Calculate the upper control limit (UCL) and lower control limit (LCL) for the averages 0f sample. At this point, the chart will look like a Run Chart. However, the uniqueness of the Control Chart becomes evident as calculate the control limits. Control limits define the parameters for determining whether a process is in statistical control. To find the X-Bar and S chart control limits, use the following formula:

Central Line for $\bar{X}$ chart $CL_{\bar{X}} = \bar{\bar{X}}$

Upper Control limit for $\bar{X}$ Chart $UCL_{\bar{X}} = \bar{\bar{X}} + A_3\bar{S}$

Lower Control limit for $\bar{X}$ Chart $LCL_{\bar{X}} = \bar{\bar{X}} - A_3\bar{S}$

Central Line for S Chart $CL_S = \bar{S}$

Upper Control limit for S Chart $UCL_S = B_4\bar{S}$

Lower Control limit for S chart $LCL_S = B_3\bar{S}$

Standard Deviation $\sigma_X = \frac{\bar{S}}{C_4}$

Where $\bar{\bar{X}}$ is the grand mean of all the individual subgroup averages $\bar{S}$ is

$A_3, B_4, B_3, C_4$ are factors of control limits reference from table 8b – table of constants for control chart

3. Mathematical model of Reactor - Heat Exchanger System

The reactor heat exchanger considered in this study is demonstrated in Figure 3.1. In RHE framework, a first request exothermic response A gives B happens. The improvement objective in the configuration of RHE framework is to focus the ideal reactor volume V and the territory of warmth exchanger A to dynamic at least 90% transformation of reactant. The imperative mathematical statements are planned by making autonomous minister material and heat balance and the heat exchanger design and energy balance.

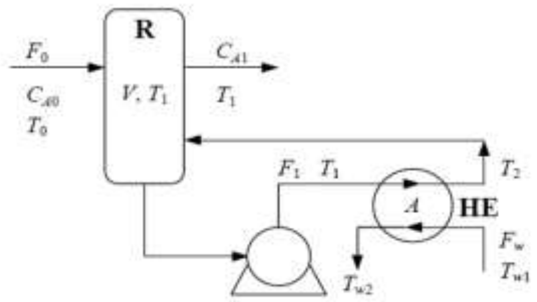



Figure 3.1 Reactor a Heat Exchanger System

Reactor Material Balance and Heat Balance

The material balance for the reactor can be written by

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

The heat balance for the reactor is given by

$$F_0 C_P (T_0 - T_1) - F_1 C_P (T_1 - T_2) + (-\Delta H_R) F_0 x_A = 0$$

Heat Exchanger Design Balance and Energy Balance

The heat exchanger design balance can be written as

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

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

$$(\Delta T_{lm}) = \frac{(T_1 - T_{w2}) - (T_2 - T_{w2})}{\ln \frac{(T_1 - T_{w2})}{(T_2 - T_{w2})}}$$

The heat exchanger energy balance is

$$F_1 C_P (T_1 - T_2) = F_w C_{P_w} (T_{w_2} - T_{w_1})$$

The temperature bounds are

$311 \le T_1 \le 389K$, $311 \le T_2 \le 389K$,
$300 \le T_{w_2} \le 380K$

The heat exchanger operation constraints are

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

$T_2 - T_{w_1} \ge 11.1$

The quality constraint is

$$x_A \ge 0.90$$

Problem Formulation for the Optimization of RHE

The design objective of RHE system is to minimize the total plant cost ($/year) including the investment and operating cost. It is given by

$$\text{Cost} = 691.2V^{0.7} + 873.6A^{0.6} + 1.76F_w + 7.056F_1$$

The initial two term of right side speaks to the speculation cost and the other two term is the working expense included in the framework. The target capacity is liable to fairness and imbalance limitations framed from the material and vitality equalization comparisons of the procedure. The consistent parameter values for RHE framework are given in Table 3.1.

Table 3.1 Parameter Values for 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) |

Solution Methodology for RHE

A penalty function methodology is utilized to handle the express limitations. Punishment terms are consolidated in the goal capacity, which lessen the wellness of the string as indicated by the size of their infringement. Mathematical statement 4.17 depicts the target capacity for the configuration of RHE framework.

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

## 4. 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. 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 | 4634.23 | 3552.467 |

| | | |
|---|---|---|
| ($/year) | | |
| Total Annual Cost ($/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.

Table4.2. Control Parameters

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

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.

## Uncertainty

At the design stage of a process system (RHE), decisions have to be made in the presence of high uncertainty level. For instance, equipment configuration and dimensions, and their operating conditions have to be decided on the basis of an available process model, whose parameters may be uncertain, and on external in formation, which commonly exhibits a random behavior. Control limit methods to quality engineering provides a robust design strategy aimed at determining nominal settings for the control variables and their associated tolerance limits, in order to reduce process sensitivity to uncertainty.

## Control Limit Chart

Firstly, the sample data are collected for the RHE system from stimulating DE. Next by adopting the procedures X bar and S control charts are generated for the four control variables such as reactant temperature after cooling, cooling water outlet temperature, reactant flow rate- heat exchanger and cooling water flow rate and summarized from the Figure 4.1 to Figure 4.4.

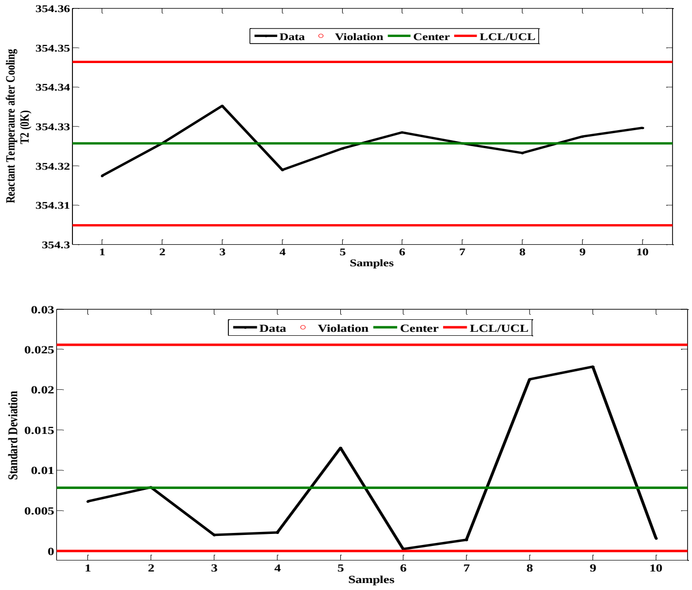



Figure 4.1 X bar and S Control Chart - Reactant Temperature after Cooling

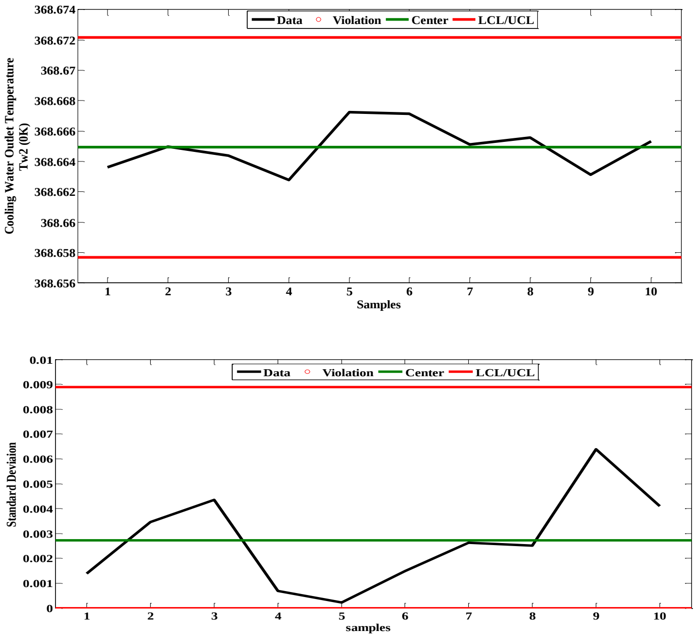
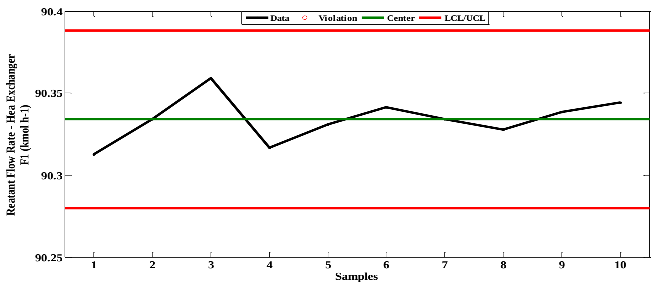



Figure 4.2 X bar and S Control Chart – Cooling Water Outlet Temperature



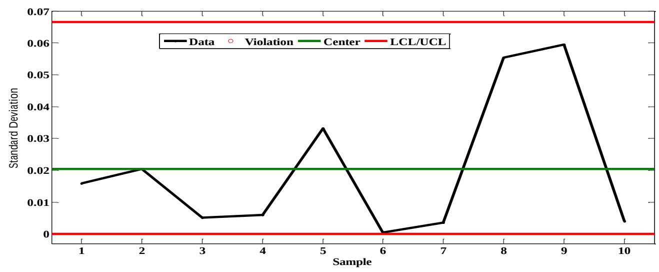
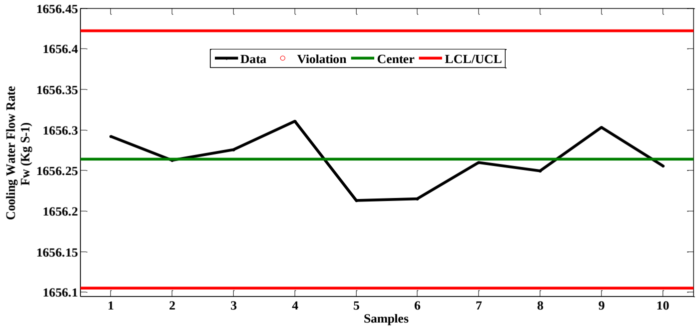



Figure 4.3 X bar and S Control Chart - Reactant Flow Rate -Heat Exchanger



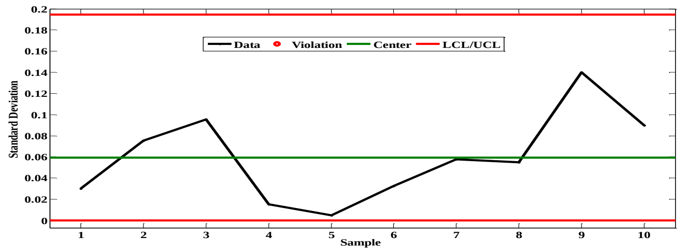




Figure 4.4 X bar and S Control Chart – Cooling Water Flow Rate

From all the X bar and S chart , it is observed that the sample data are falls within the upper control and lower control limit of the operating point of the RHE system and the system is in control limit

## 6 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.To determining nominal settings for the control variables and their associated tolerance limits, in order to reduce process sensitivity to uncertainty

## Reference

[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.

[11] Gopalakrishnan.B, P.K.Bhaba. "Computation of the Optimal Value of Operating Parameters in a Reactor – Heat Exchanger System by Differential Evolution Techniques", International Journal of Recent Technology and Engineering, Vol 1 (6), 2013, pp 2277-3878.

[12] John J. Flaig and Fred Khorasani, (2013), "Process Capability Analysis using Curve Fitting Methods", Global Journal of Researches in Engineering, General Engineering, Vol. 13(2) Ver 1.0.

[13] John J. Flaig and William C. Spencer, (2006), "Process Qualification", Quality Engineering, Vol. 16(1), PP 57.

[14] John J. Flaig, (2002), "Process Capability Optimization", Quality Engineering, Vol. 15(2), PP 233.

[15] John J. Flaig, (2006) "Selecting Optimal Specification Limits", Quality Technology & Quantitative Management, Vol. 3(2), PP 207.