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Optimal Design of William – Otto Process Plant Using Differential Evolution Algorithm

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Abstract: Evolutionary computation is an artificial intelligence technique based on the principle of natural selection and natural genetics. The optimal design of process plant is complex and it involves multitude of equality and inequality constraints. In this study, an optimal design of William-Otto (WO) process plant is carried out using Differential Evolution algorithm (DE). The design problem is selected as it resembles the real time optimal design of process plants. From the optimal design results, it is noticed that differential evolution outperforms the other methodologies. It is concluded that DE gives the most reliable and robust technique for the optimization of process plants.
Keywords: optimal design, evolutionary computation, differential evolution algorithm, WO process plant.

Introduction

Optimization methods coupled with modern tools of computer-aided design are used to enhance the creative process of conceptual and detailed design of engineering system. Optimization problems are to be handled by a suitable and reliable optimization tool, which integrates the entire process steps by a single global optimization approach. Evolutionary computing is a rapidly growing area of artificial intelligence.

The design of Williams Otto process plant (WO) process had been studied with variety of optimization techniques in several literature[1-10]. These techniques suffer from many drawbacks that include requirement of significant computational effort in the formulation of problem, inefficiency in handling the equality constraints, requirement of good starting values for the search and are found to be unsuitable for unbounded/non-convex natured problems. It has been proved that the optimal design of process plant can be effetely achieved by the use of Genetic Algorithm[11]. In the present study, Differential Evolutionary techniques have been used to optimize the Williams Otto process plant (WO) which represents difficult non-linear optimization with the equality and inequality constraints.

Differential Evolution

Differential Evolution (DE) is an improved version of genetic algorithm. 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 searches. 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[12]. The DE algorithm[13] is described as follows:

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

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

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

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

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, this amount is subtracted or added to the limit violated to shift the value inside the limits.

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.
$$\hat{Z}_i^{G+1} = \begin{cases} Z_{ji}^G, & \text{if a random number} > C_R \\ \hat{Z}_{ji}^{G+1}, & \text{otherwise} \end{cases} \qquad i = 1 \ldots N_P,\ j = 1 \ldots n \tag{3}$$

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

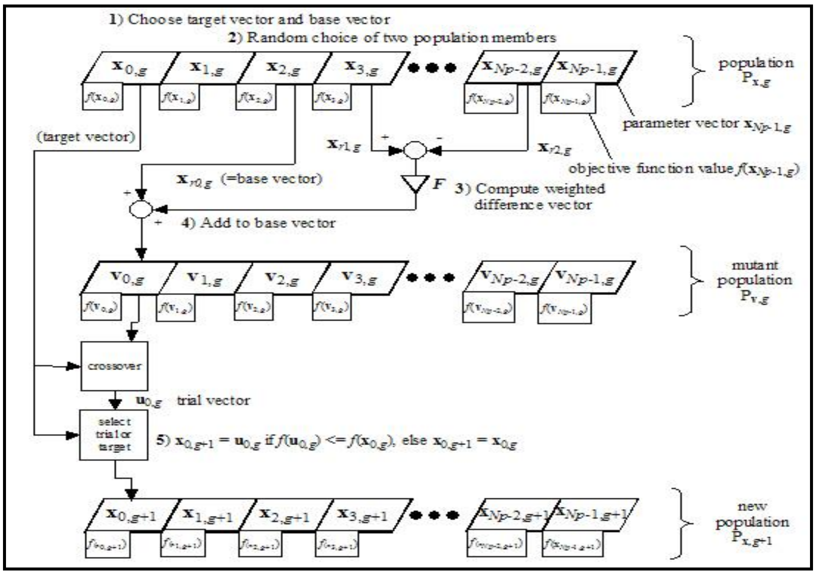
Evaluation and Selection

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. Contrarily 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

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

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

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. Figure1 shows the steps involved in basic differential evolution.



DE is advantageous as the minimization method 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[13].

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.

Williams - Otto Process Plant

This problem addresses design optimization of Williams – Otto process plant as shown in Figure 2.

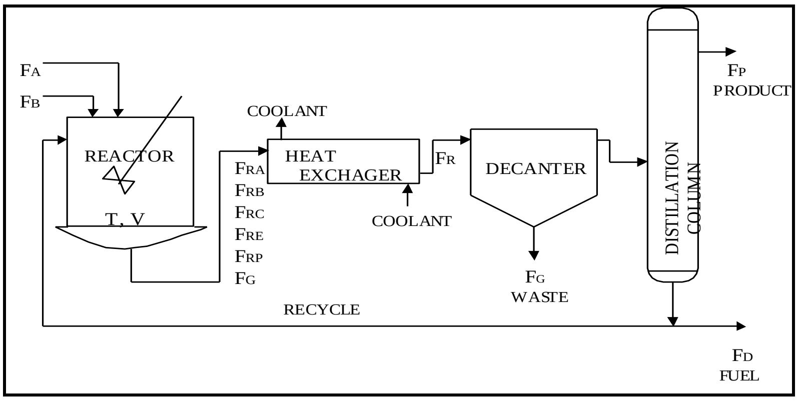


Fig.2. Williams - Otto process plant

WO plant consists of a stirred tank reactor and separation system consisting of heat exchanger, decanter and distillation column. The plant is built to manufacture 0.6 kg/s of the distillate product P. The rate of reaction is found to be negligible below 70ºC and substantial decomposition occurs above 110 ºC. In the reactor, three exothermic second order reactions take place and are represented by the equations 6 to 8

$$A + B \xrightarrow{k_1} C \quad (6)$$

$$C + B \xrightarrow{k_2} P + E \quad (7)$$

$$P + C \xrightarrow{k_3} G \quad (8)$$

The reaction coefficient of each individual reaction is represented by the classical Arrhenius form

$$k_i = U_i \exp\left(-F_i / T\right) \quad (9)$$

where

$U_1 = 5.9755 \times 10^{9}\, h^{-1}$., weight fraction A or B

$U_2 = 2.5962 \times 10^{12}\, h^{-1}$., weight fraction B

$U_3 = 9.6283 \times 10^{15}\, h^{-1}$., weight fraction C

$F_1 = 6{,}666.67\ K$

$F_2 = 8{,}333.33\ K$

$F_3 = 11{,}111.11\ K$

The reactor effluent contains six components; the flow rates of the raw materials A and B, the desired product P which is to removed by distillation, an intermediate compound C and E and byproduct G. The inert material G is heavy oil becomes an insoluble in the effluent after the effluent stream is cooled, separated in the decanter and disposed of as a waste material. This waste treatment step incurs additional cost to the overall process plant. The recovery of desired product P will be incomplete as it forms an azeotropic mixture with the bottoms of the distillation column. Discarding a portion of the bottom product controls concentration of inert and others are recycled to the reactor. The reaction rates of the second order irreversible reactions taking place in WO plant are given by

$$r_1^* = k_1 F_{RA} F_{RB} \frac{V\rho}{F_R^2} \quad (10)$$

$$r_2^* = k_2 F_{RB} F_{RC} \frac{V\rho}{F_R^2} \quad (11)$$

$$r_3^* = k_3 F_{RP} F_{RC} \frac{V\rho}{F_R^2} \quad (12)$$

The constraint equations are formulated by making independent material balances across the system, by a constraint on separation efficiency in the distillation column and by the definition of the total rate from the reactor.

Optimization Problem Formulation

The objective of the optimization of Williams -Otto plant is to maximize the percent return on investment. The percent return on investment is defined as the ratio of operating profit and total investment and is given by

$$P^* = \left(\frac{1}{6V\rho}\right)\left(84F_A - 201.96F_D - 336F_G + 1955.52F_P - 2.22F_R - 60V\rho\right) \quad (13)$$

The objective function is subject to the equality constraints formed from the material balance equations of the process.

Overall Material Balance

$$G_1^* = F_A + F_B - F_G - F_P - F_D = 0 \tag{14}$$

Constraint on the Separation Efficiency of the Distillation Column

$$G_2^* = F_{RP} - 0.1 F_{RE} - F_P = 0 \tag{15}$$

Material Balance on Component E

$$G_3^* = \left(\frac{M_E}{M_B}\right) k_2 \left(\frac{F_{RB} F_{RC}}{F_R^2}\right) V\rho - F_D \left(\frac{F_{RE}}{F_R - F_G - F_P}\right) = 0 \tag{16}$$

Material Balance on Component P

$$G_4^* = \left[k_2 F_{RB} F_{RC} - \left(\frac{M_P}{M_C}\right) k_3 F_{RC} F_{RP} \right] \frac{V\rho}{F_R^2} - F_D \left(\frac{F_{RP} - F_P}{F_R - F_G - F_P}\right) - F_P = 0 \tag{17}$$

Material Balance on Component A

$$G_5^* = \left(- k_1 F_{RA} F_{RB}\right) \frac{V\rho}{F_R^2} - F_D \left(\frac{F_{RA}}{F_R - F_P - F_G}\right) + F_A = 0 \tag{18}$$

Material Balance on Component B

$$G_6^* = \left(- k_1 F_{RA} F_{RB} - k_2 F_{RB} F_{RC}\right) \frac{V\rho}{F_R^2} - F_D \left(\frac{F_{RB}}{F_R - F_P - F_G}\right) + F_B = 0 \tag{19}$$

Material Balance on Component C

$$G_7^* = \left[\left(\frac{M_C}{M_B}\right) k_1 F_{RA} F_{RB} - \left(\frac{M_C}{M_B}\right) k_2 F_{RB} F_{RC} - k_3 F_{RP} F_{RC} \right] \frac{V\rho}{F_R^2} - F_D \left(\frac{F_{RC}}{F_R - F_G - F_P}\right) = 0 \tag{20}$$

Material Balance on Component G

$$G_8^* = \left(\frac{M_G}{M_C}\right) k_3 F_{RC} F_{RP} \frac{V\rho}{F_R^2} - F_G = 0 \tag{21}$$

Definition of Total Flow Rate from the Reactor

$$G_9^* = F_{RA} + F_{RB} + F_{RC} + F_{RE} + F_G + F_{RP} - F_R = 0 \tag{22}$$

The optimization study of Williams -Otto chemical plant consists of twelve process variables which have influence on the percent return on investment and the variables are F_A, F_B, F_D, F_G, F_R, F_P, F_{RA}, F_{RB}, F_{RC}, F_{RE}, F_{RP}, V and T. Process variables in WO plant are highly nonlinear. The equality constraints formed from the material balance equations pose difficulties in locating the optimum values.

* The original problem formulation is in FPS units.

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 equation 23 describes the objective function for the design of WO plant.

Maximize

$$\psi^* = \left(\frac{84F_A - 201.96F_D - 336F_G + 1955.52F_P - 2.22F_R - 60V\rho}{6V\rho}\right) - \lambda \times \sum_{z=1}^{9} \left| G_z{}^S - G_z \right| \tag{23}$$

Subject to

$$\sum_{z=1}^{9} G_Z = 0 \tag{24}$$

$$F_P \geq 0.6 \ \text{kg/s} \tag{25}$$

$$70 \leq T \leq 110 \ ^{\circ}C \tag{26}$$

Results and Discussion

The results obtained using DE for the design optimization of the WO process plant. The optimal design results in S.I. units (based on DE) are also noticed in the WO process plant (Refer Table 1; P% =121.7 & CPU time =0.1s). As the investment cost is directly proportional to the mass of the reactor (600 Vρ), the reduction in reactor volume requirement has a significant bearing on the outcome of the economics of the plant.

Table 1: Performance analysis of DE based optimal design with other Evolutionary Techniques –WO process plant

Variables	GA	DE
F_A (kg/s)	1.7075	1.701
F_B (kg/s)	3.8730	3.878
F_D (kg/s)	4.5759	4.575
F_G (kg/s)	0.4045	0.405
F_P (kg/s)	0.6001	0.6001
F_R (kg/s)	47.3497	46.663
F_{RA} (kg/s)	6.1223	5.975
F_{RB} (kg/s)	18.7498	18.531
F_{RC} (kg/s)	1.0031	0.9792
F_{RE} (kg/s)	18.6090	18.339
F_{RP} (kg/s)	2.4610	2.434
T ^{o}c	101.54	101.539
V m^3	0.8647	0.8706
P %	121.54	121.7
CPU Time (s)	0.5	0.1

From the results, it is inferred that DE based optimization is found to be more successful in optimal design of WO plant. DE predicated design increases the percentage return on investment by maximum fine tuning of design variables.

In all the three cases, the computational works are carried out in the platform of C++ in Core (TM) Due 1.66 GHz processor. In addition, evolutionary computation parameters employed in this works are furnished in Table 2.

Table 2: Computational parameters

Control parameters	Symbol	value
Population of each generation	NP	20
Weight Applied to Random Differential	F	0.65
Crossover Constant	C_R	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.

Conclusions

This paper demonstrates the successful application of Evolutionary algorithms for the optimal design of WO process plant. The result of the work indicates that DE is found to be better techniques than the genetic algorithm. DE can be considered as a complement to the global optimization techniques. DE based optimal design does not require complicated mathematical formulations and efficient in handling problems with large number of discrete variables and constraints.

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