Design Optimization of Process Plants Using Real Coded Genetic Algorithm

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The application of artificial intelligence based search and optimization algorithms is an active research area in many engineering fields. In this work, real coded genetic algorithm, a modified genetic algorithm is used for the optimal design of industrial process plants. This technique has been implemented for the optimal design of reactor network, Williams-Otto process plant and multiproduct process plant. The modification to simple genetic algorithm, using real coded representation of variables along with specifically designed mutation and crossover operator, yields accurate results for the problems considered in this paper, at a lesser computational effort. The results have been compared with the conventional and global optimization techniques. The simulation study clearly demonstrates that the proposed real coded genetic algorithm is practical, robust, and reliable optimization technique for the design of industrial process plants.

Key words:
Optimal design, Real coded genetic algorithm, Reactor network, Williams-Otto plant, Multiproduct Process.

Introduction

Optimization methods coupled with modern tools of computer–aided design are also being 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. Genetic algorithm is a part of evolutionary computing, which is a rapidly growing area of artificial intelligence. GA is an optimization algorithm based on the mechanics of natural selection and natural genetics. It combines solution evaluation with randomized, structured exchange of information between the solutions to obtain optimality. GA is a robust approach as there is no restriction on the solution space during the search.

In the present study real coded genetic algorithm (RCGA) has been used to solve the three chemical engineering problems viz. (i) Optimal design of CSTRs in series for consecutive reaction, (ii) Design optimization of Williams Otto process plant and (iii) Design optimization of multiproduct process plant. These problems represent difficult non–linear optimization problems, with the equality and inequality constraints.

The optimal design of reactor network constitutes a very difficult test problem, studied for the evaluation global optimization techniques as found in literature.[1,2,3] It possesses a local minimum with an objective function value that is very close to that of the global solution.

The design of WO process had been studied with variety of optimization techniques in several literature.[4–12] 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.

Several optimization techniques have been reported in the literature for the least–cost design of multiproduct process. The optimal design of multiproduct process plants was carried out by conventional techniques[13,14] that make use of algorithm devised for solving general optimization problems. These algorithms are most effective for moderately constrained optimization problems with continuous decision variables, whereas the multiproduct process design consists of discrete and continuous decision variables and involves large number of constraints.

Heuristic method was also reported for the design of multiproduct process plants.[15,16] However this method may end up in local optimum because of its greedy nature. Mixed integer linear programming (MILP) and mixed integer nonlinear programming (MINLP) techniques were also used in the design of process plants. The methods of problem formulation using MILP and MINLP had strong influ-

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ence on evaluation procedure and in quality of results.[17] Hence, it is very clear that all these methods require rigorous, tedious and laborious computations.

Several optimization algorithms like GRG2, SQP, QP, Powell's algorithm and Nelder –Mead algorithm can be used for the process plant design optimization and control. Among them the constrained non–linear technique has eminent benefits for explicit handling of the constraints, fast convergence and numerical stability.[18] It was proved that Nelder Mead algorithm requires a good starting point and in continuous process operations it is not possible to predict the suitable starting point to obtain the optimum design value. This technique lands at the local optimum values nearer to the initial guess of design variables.[19] GA based design optimization methodology overcomes the shortcomings of the conventional search methods as it starts with a population representing many points. Therefore, an exceptionally simple evolutionary computation method, RCGA, is significantly faster and yields the global optimum for the problems considered in the present study.

Genetic algorithm

Genetic algorithm operates on several solutions simultaneously, gathering information from current search points and using it to direct subsequent searches, that make GA less susceptible to land at local optimum values. GA offers significant savings in computational effort by selectively searching a much smaller fraction of the solution space for problems involving large number of discrete variables. It exploits efficiently historical information to speculate on new search points with expected improved performance. GA is just such a technique, an intelligent way to search for the optimum solution to problem hidden in a wealth of poorer ones.[20] GA is proven to be an efficient technique in solving the chemical engineering design problems. Traditional GA uses the binary representation that eventually discretizes a real design space and suffer from disadvantages, when applied to the real world design problems. A simple solution to these problems can be obtained by the use of real coded genetic algorithm with floating–point representation of variables. The present approach has been found to be robust, accurate, and efficient, as the floating–point representation is conceptually closest to the real design space.[21]

Real coded genetic algorithm

In real coded GA, an individual is coded as a vector of real numbers corresponding to the design variables. The genetic operations i.e., mutation and crossover in this case do not handle bit strings and are defined in a different manner, for example mutation operation does not randomly change one bit but randomly chooses a floating point number within a particular range.[22] In this approach, the operating scope of genetic operators is dynamic. It is time dependent and depends on the number of generations or iterations. The goal at the beginning of the process is rough location of the global optimum. As the process develops, increasing the operating scope of the operators enables fine local tuning of the solution. The crossover operators employed in this work include simple crossover, arithmetic crossover and heuristic crossover[23] with a combination of binary mutation, multi non–uniform mutation and boundary mutation.

Case studies

Problem 1: Global optimization of reactor network design

The real coded genetic algorithm has been applied for the optimal design of two CSTRs in series, for a consecutive reaction $A \rightarrow B \rightarrow C$. The concentration of B in the outlet stream of the second reactor needs to be minimized subject to an upper bound on the investment cost. Reactions taking place in this system follows the first order kinetics. The kinetic coefficients are

$$k_{11} = 9.755988 \times 10^{-2}\ \mathrm{s}^{-1};$$

$$k_{21} = 3.919080 \times 10^{-2}\ \mathrm{s}^{-1};$$

$$k_{12} = 9.658428 \times 10^{-2}\ \mathrm{s}^{-1};$$

$$k_{22} = 3.527172 \times 10^{-2}\ \mathrm{s}^{-1}.$$

The inlet concentration is $c_{\mathrm{A}_0} = 1.0$ mol l^{-1} and the inlet concentration for, both, B and C is zero.

Optimization problem formulation

The reactor design problem can be formulated as the following non–convex optimization problem.

Minimize

$$-c_{\mathrm{B}_2} \tag{1}$$

subject to

$$(C_{\mathrm{A}_1} - C_{\mathrm{A}_0}) + k_{11} c_{\mathrm{A}_1} v_1 = 0 \tag{2}$$

$$(C_{\mathrm{A}_2} - C_{\mathrm{A}_1}) + k_{12} c_{\mathrm{A}_1} v_2 = 0 \tag{3}$$

$$(C_{\mathrm{B}_1} + C_{\mathrm{A}_1} - C_{\mathrm{A}_0}) + k_{21} c_{\mathrm{B}_1} v_1 = 0 \tag{4}$$

$$(C_{B_2} - C_{B_1} + C_{A_2} - C_{A_1}) + k_{22} c_{B_2} v_2 = 0 \quad (5)$$

$$\tau_1^{0.5} + \tau_2^{0.5} \le 4.0 \quad (6)$$

$$0 \le c_{A_1}, c_{B_1}, c_{A_2}, c_{B_2} \le 1.0 \quad (7)$$

$$0 \le V_1, V_2 \le 100 \quad (8)$$

The capital cost of a reactor is proportional to the square root of its residence time; the constraint provides an upper bound on the total investment costs. The problem constitutes a very difficult test problem, as it possesses a local minimum with an objective function value, that is very close to that of the global solution.[1]

Problem 2: Williams-Otto process plant

This problem addresses design optimization of Williams-Otto (WO) process plant as in Figure 1. WO plant consists of a stirred tank reactor and separation system consisting of heat exchanger, decanter and distillation column.[4] The plant is built to manufacture 0.6 kg s^{-1} of the distillate, product P. The rate of reaction is found to be negligible below 70 °C and substantial decomposition occurs above 110 °C. In the reactor, three exothermic second order reactions take place and are represented by the equations 9 to 11.

$$A + B \xrightarrow{k_1} C \quad (9)$$

$$C + B \xrightarrow{k_2} P + E \quad (10)$$

$$P + C \xrightarrow{k_3} G \quad (11)$$

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

$$k_i = k_{i_0} \exp(-F_i / T) \quad (12)$$

where

$$k_{10} = 5.9755 \times 10^9 \text{ h}^{-1}, \text{ fraction A or B}$$

$$k_{20} = 2.5962 \times 10^{12} \text{ h}^{-1}, \text{ fraction B}$$

$$k_{30} = 9.6283 \times 10^{15} \text{ h}^{-1}, \text{ fraction A}$$

$$F_1 = 6\ 666.67 \text{ K}$$

$$F_2 = 8\ 333.33 \text{ K}$$

$$F_3 = 11\ 111.11 \text{ K}$$

The reactor effluent contains six components; the flow rates of the raw materials A and B, the desired product P which is 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

$$\gamma_1^* = k_1 q_{RA} q_{RB} \frac{V \rho}{q_R^2} \quad (13)$$

$$\gamma_2^* = k_2 q_{RB} q_{RC} \frac{V \rho}{q_R^2} \quad (14)$$

$$\gamma_3^* = k_3 q_{RP} q_{RC} \frac{V \rho}{q_R^2} \quad (15)$$

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.

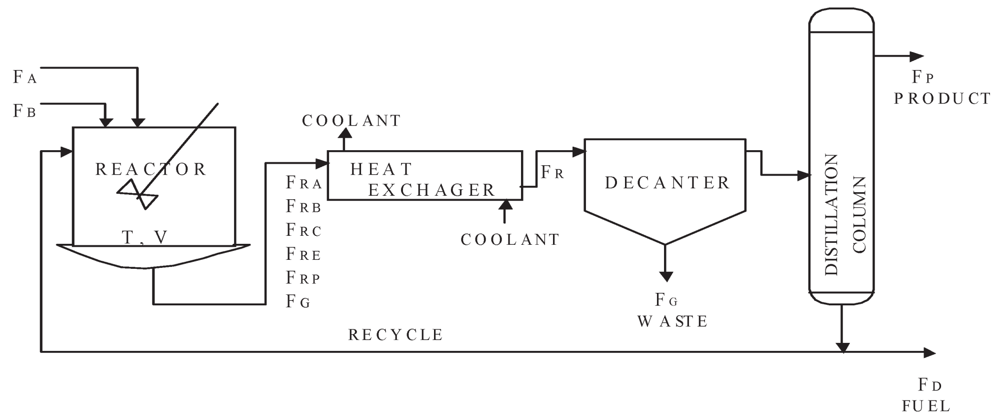

Fig. 1 – *Williams-Otto Process Plant*

Optimization problem formulation

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

$$P^{*}=\left(\frac{1}{6V\rho}\right)(84q_{\mathrm{A}}-201.96q_{\mathrm{D}}-336q_{\mathrm{G}}+ +1955.52q_{\mathrm{P}}-2.22q_{\mathrm{R}}-60V\rho) \tag{16}$$

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

Overall Material Balance

$$G_{1}^{*}=q_{\mathrm{A}}+q_{\mathrm{B}}-q_{\mathrm{G}}-q_{\mathrm{P}}-q_{\mathrm{D}}=0 \tag{17}$$

Constraint on the Separation Efficiency of the Distillation Column

$$G_{2}^{*}=q_{\mathrm{RP}}-0.1q_{\mathrm{RE}}-q_{\mathrm{P}}=0 \tag{18}$$

Material Balance on Component E

$$G_{3}^{*}=\left(\frac{M_{\mathrm{E}}}{M_{\mathrm{B}}}\right)k_{2}\left(\frac{q_{\mathrm{RB}}q_{\mathrm{RC}}}{F_{\mathrm{R}}^{2}}\right)V\rho- -q_{\mathrm{D}}\left(\frac{q_{\mathrm{RE}}}{q_{\mathrm{R}}-q_{\mathrm{G}}-q_{\mathrm{P}}}\right)=0 \tag{19}$$

Material Balance on Component P

$$G_{4}^{*}=\left[k_{2}q_{\mathrm{RB}}q_{\mathrm{RC}}-\left(\frac{M_{\mathrm{P}}}{M_{\mathrm{C}}}\right)k_{3}q_{\mathrm{RC}}q_{\mathrm{RP}}\right]\frac{V\rho}{F_{\mathrm{R}}^{2}}- -q_{\mathrm{D}}\left(\frac{q_{\mathrm{RP}}-q_{\mathrm{P}}}{q_{\mathrm{R}}-q_{\mathrm{G}}-q_{\mathrm{P}}}\right)-q_{\mathrm{P}}=0 \tag{20}$$

Material Balance on Component A

$$G_{5}^{*}=(-k_{1}q_{\mathrm{RA}}q_{\mathrm{RB}})\frac{V\rho}{F_{\mathrm{R}}^{2}}- -q_{\mathrm{D}}\left(\frac{q_{\mathrm{RA}}}{q_{\mathrm{R}}-q_{\mathrm{P}}-q_{\mathrm{G}}}\right)+q_{\mathrm{A}}=0 \tag{21}$$

Material Balance on Component B

$$G_{6}^{*}=(-k_{1}q_{\mathrm{RA}}q_{\mathrm{RB}}-k_{2}q_{\mathrm{RB}}q_{\mathrm{RC}})\frac{V\rho}{F_{\mathrm{R}}^{2}}- -q_{\mathrm{D}}\left(\frac{q_{\mathrm{RB}}}{q_{\mathrm{R}}-q_{\mathrm{P}}-q_{\mathrm{G}}}\right)+q_{\mathrm{B}}=0 \tag{22}$$

Material Balance on Component C

$$G_{7}^{*}=\left[\left(\frac{M_{\mathrm{C}}}{M_{\mathrm{B}}}\right)k_{1}q_{\mathrm{RA}}q_{\mathrm{RB}}-\left(\frac{M_{\mathrm{C}}}{M_{\mathrm{B}}}\right)k_{2}q_{\mathrm{RB}}q_{\mathrm{RC}}- -k_{3}q_{\mathrm{RP}}q_{\mathrm{RC}}\right]\frac{V\rho}{q_{\mathrm{R}}^{2}}-q_{\mathrm{D}}\left(\frac{q_{\mathrm{RC}}}{q_{\mathrm{R}}-q_{\mathrm{P}}-q_{\mathrm{G}}}\right)=0 \tag{23}$$

Material Balance on Component G

$$G_{8}^{*}=\left(\frac{M_{\mathrm{G}}}{M_{\mathrm{C}}}\right)k_{3}q_{\mathrm{RC}}q_{\mathrm{RP}}\frac{V\rho}{F_{\mathrm{R}}^{2}}-q_{\mathrm{G}}=0 \tag{24}$$

Definition of Total Flow Rate from the Reactor

$$G_{9}^{*}=q_{\mathrm{RA}}+q_{\mathrm{RB}}+q_{\mathrm{RC}}+q_{\mathrm{RE}}+ +q_{\mathrm{G}}+q_{\mathrm{RP}}-q_{\mathrm{R}}=0 \tag{25}$$

The optimization study of Williams-Otto chemical plant consists of twelve process variables which have influence on the percentange (%) return on investment and the variables are q_{A}, q_{B}, q_{D}, q_{G}, q_{R}, q_{P}, q_{RA}, q_{RB}, q_{RC}, q_{RE}, q_{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.

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 26 describes the objective function for the design of WO plant.

Maximize

$$\Psi^{*}=\left(\frac{84q_{\mathrm{A}}-201.96q_{\mathrm{D}}-336q_{\mathrm{G}}+1955.52q_{\mathrm{P}}-2.22q_{\mathrm{R}}-60V\rho}{6V\rho}\right)- -\lambda\times\sum_{z=1}^{9}|G_{z}^{S}-G_{z}| \tag{26}$$

Subject to

$$\sum_{z=1}^{9}G_{z}=0 \tag{27}$$

$$q_{\mathrm{P}}\geq 0.6\ \mathrm{kg\ s^{-1}} \tag{28}$$

$$70\leq T\leq 110\ °\mathrm{C} \tag{29}$$

* The original problem formulation is in FPS units.

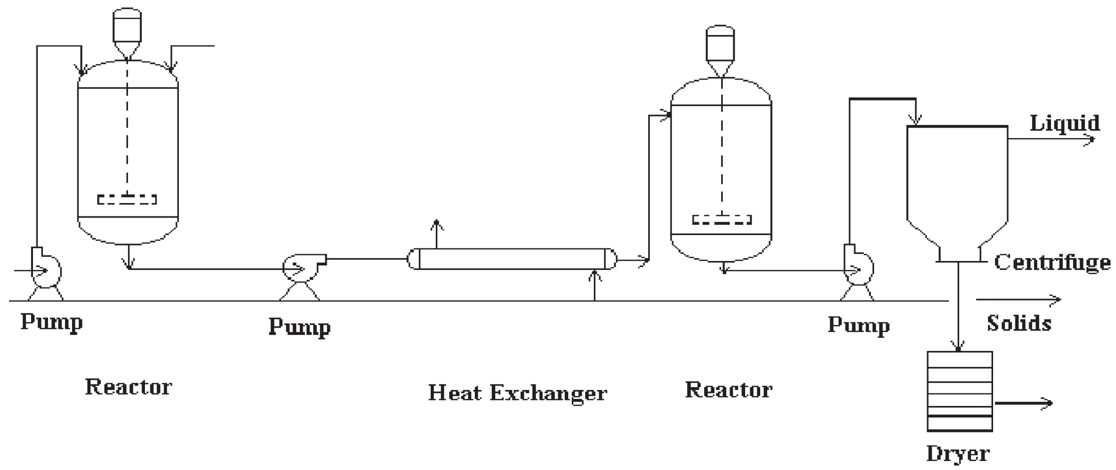

Fig. 2 – *Multiproduct industrial process plant*

Problem 3: Multiproduct industrial process

The process shown in Figure 2 consists of three batch units: two reactors and a dryer and five semi-continuous units, three pumps, one heat exchanger and one centrifuge[13]. It is to process three products over a planning horizon of one year of about 8000 h. The production requirements and the batch processing times of each product in batch units are given in Table 1. All three products are to be processed serially in all units, with the exception that product 2 will by-pass reactor 2 and be sent directly to the centrifuge. The volume of material that must be processed at each stage to produce one kg of final product differs for different products. The volume factors for the three products and eight units are given in Table 2. For batch units the equipment cost is given by a power law correlation of the form $a_i V_i^{\alpha_1}$. Semi–continuous unit costs are represented as $b_j Q_j^{\beta_j}$. The cost coefficients for eight equipments are given in Table 3.

Table 1 – *Multiproduct process – production requirements and batch processing time*

Products	Production requirements kg y^{-1}	Batch processing time, hr		
		reactor 1	reactor 2	dryer
product 1	400000	3	1	4
product 2	300000	6	–	8
product 3	100000	2	2	4

Table 2 – *Multiproduct process – massic volume / m^3 kg^{-1} of final product*

	Equipment	Product 1	Product 2	Product 3
Batch units	reactor 1	1.2	1.5	1.1
	reactor 2	1.4	–	1.2
	dryer	1.0	1.0	1.0
Continuous units	pump1	1.2	1.5	1.1
	pump 2	1.2	1.5	1.1
	heat exchanger	1.2	1.5	1.1
	pump 3	1.4	–	1.2
	centrifuge	1.4	1.5	1.2

Table 3 – *Multiproduct process – cost coefficients*

Equipment	Batch unit		Continuous unit	
	a_i	α_i	b_j	β_j
reactor 1	592	0.65		
reactor 2	582	0.39		
dryer	1200	0.52		
pump 1			370	0.22
pump 2			250	0.40
heat exchanger			210	0.62
pump 3			250	0.40
centrifuge			200	0.83

Optimization problem formulation

The capital cost of multiproduct process to be minimized is given by the equation

$$f = \Sigma a_i V_i^{\alpha_i} + \Sigma b_i Q_j^{\beta_j} \tag{30}$$

subject to the following constraints:

Total time constraint:

$$\frac{400\,000}{S_1} t_1 + \frac{300\,000}{S_2} t_2 + \frac{100\,000}{S_3} t_3 \leq 8000 \tag{31}$$

Reactor 1 volume constraints:

$$V_1 \geq 1.2\,S_1 \quad V_1 \geq 1.5\,S_2 \quad V_1 \geq 1.1\,S_3 \tag{32}$$

Reactor 2 volume constraints:

$$V_2 \geq 1.4\,S_1 \qquad V_2 \geq 1.2\,S_3 \tag{33}$$

Dryer volume constraints:

$$V_3 \geq 1.0\,S_1 \quad V_3 \geq 1.0\,S_2 \quad V_3 \geq 1.0\,S_3 \tag{34}$$

Cycle time of Product 1:

$$\begin{aligned} t_1 &\geq \frac{1.2\,S_1}{Q_1} + 3 + \frac{1.2\,S_1}{Q_2} && \text{Reactor 1} \\ t_1 &\geq \frac{1.2\,S_1}{Q_3} + 1 + \frac{1.4\,S_1}{Q_4} && \text{Reactor 2} \\ t_1 &\geq \frac{1.4\,S_1}{Q_5} + 4 && \text{Dryer} \end{aligned} \tag{35}$$

Cycle time of Product 2:

$$\begin{aligned} t_2 &\geq \frac{1.5\,S_2}{Q_1} + 6 + \frac{1.5\,S_2}{Q_2} && \text{Reactor 1} \\ t_2 &\geq \frac{1.5\,S_2}{Q_5} + 8 && \text{Dryer} \end{aligned} \tag{36}$$

Cycle time of Product 3:

$$\begin{aligned} t_3 &\geq \frac{1.1\,S_3}{Q_1} + 2 + \frac{1.1\,S_3}{Q_2} && \text{Reactor 1} \\ t_3 &\geq \frac{1.1\,S_3}{Q_3} + 2 + \frac{1.2\,S_3}{Q_4} && \text{Reactor 2} \\ t_3 &\geq \frac{1.1\,S_3}{Q_5} + 4 && \text{Dryer} \end{aligned} \tag{37}$$

Consecutive Semi–continuous units 2 and 3 constraints:

$$\begin{aligned} \frac{1.2\,S_1}{Q_2} &\geq \frac{1.2\,S_1}{Q_3} && \text{Product 1} \\ \frac{1.5\,S_2}{Q_2} &\geq \frac{1.5\,S_2}{Q_3} && \text{Product 2} \\ \frac{1.1\,S_3}{Q_2} &\geq \frac{1.1\,S_3}{Q_3} && \text{Product 3} \end{aligned} \tag{38}$$

Consecutive Semi–continuous units 4 and 5 constraints:

$$\frac{1.4\,S_1}{Q_4} \geq \frac{1.2\,S_1}{Q_5} \qquad \text{Product 1} \tag{39}$$

$$\frac{1.2\,S_1}{Q_4} \geq \frac{1.2\,S_3}{Q_5} \qquad \text{Product 3}$$

For product 2, the heat exchanger will feed directly to the centrifuge,

$$\frac{1.5\,S_2}{Q_2} \geq \frac{1.5\,S_2}{Q_5} \tag{40}$$

Pump flow rate constraints:

$$Q_3 \geq 1.0\,Q_2 \quad Q_5 \geq 1.0\,Q_4 \quad Q_5 \geq 1.0\,Q_2 \tag{41}$$

The optimization of multiproduct process, a nonlinear problem, consists of fourteen variables, both, discrete and continuous. The variables are three, each of cycle time of products, size, volume of batch equipments, and five volumetric flow rates in continuous equipments. The optimization problem is subjected to twenty-six inequality constraints as described by the equations (31) to (41).

Solution methodology

The objective function is to minimize

$$\psi = \sum_{i=1}^{3} a_i V_i^{\alpha_i} + \sum_{j=1}^{5} b_j Q_j^{\beta j} + \lambda \left[\sum_{z \in \mathrm{LVC}}^{26} |c_z - c_{z_{(\mathrm{limit})}}| \right] \tag{42}$$

The fitness function is formulated by the minimization function subjected to various constraints governing the process.

Results and discussion

The results obtained using real coded genetic algorithm for the global design optimization of reaction network have been compared with the Branch & Reduce algorithm, Branch & Bound algorithm, and αBB algorithm in Table 4. It is found that the proposed approach, significantly simpler, lands at the global optimum value. Hence, optimization using real coded genetic algorithm can be considered complement to global optimization techniques.

The optimum design variables of WO process plant obtained by real coded GA in S.I. units have been compared with the values obtained in earlier investigations and are furnished in Table 5. From the results it is inferred that GA based optimization study has been found to be successful in optimal design of WO process plant and values obtained are comparable to those obtained in previous investigations. GA predicated design values utilize relatively lesser reactor volume when compared to other values at the same production rate, which significantly

Table 4 – *Comparison of RCGA with global optimization algorithms – Problem 1*

Variables	Branch & bound algorithm	Branch & reduce algorithm	αBB algorithm	RCGA
c_{A_1} mol l^{-1}	0.771462	0.771462	0.771462	0.771462
c_{B_1} mol l^{-1}	0.516997	0.516997	0.516997	0.516997
c_{A_2} mol l^{-1}	0.204234	0.204234	0.204234	0.204234
c_{B_2} mol l^{-1}	0.388812	0.388812	0.388812	0.388812
V_1 l	3.037	3.036504	3.036504	3.036504
V_2 l	5.096	5.096052	5.096052	5.096052
objective function	– 0.388812	– 0.388812	– 0.388812	– 0.388812

Table 5 – *Comparison of RCGA with conventional optimization algorithms – Problem 2*

Variables	Complex method	direct search method	geometric programming	method of multipliers	RCGA
q_A	1.7020	1.7030	1.7016	1.7030	1.7075
q_B	3.8626	3.8785	3.8785	3.8785	3.8730
q_D	4.5642	4.5765	4.5753	4.5765	4.5759
q_G	0.4002	0.4048	0.4048	0.4048	0.4045
q_P	0.6001	0.6001	0.6001	0.6001	0.6001
q_R	45.4993	46.7986	46.6711	46.7986	47.3497
q_{RA}	5.8660	6.0032	5.9722	6.0032	6.1223
q_{RB}	17.9905	18.5763	18.5266	18.5763	18.7498
q_{RC}	0.9733	0.9839	0.9819	0.9837	1.0031
q_{RE}	17.8809	18.3910	18.3451	18.3910	18.6090
q_{RP}	2.3883	2.4394	2.4346	2.4394	2.4610
T	100.52	101.54	99.09	101.54	101.54
V	0.9093	0.8696	0.8707	0.8696	0.8647
P	121.33	121.53	121.53	121.53	121.54

reduces the capital cost involved in the process. As the investment cost is directly proportional to the mass of the reactor (600V q), the reduction in reactor volume requirement has a significant bearing on the outcome of the economics of the plant.

The optimal design variables of the multi-product process plant have been compared with Generalized Reduced Gradient (GRG) method and NLP technique. The details of the optimum design values have been furnished in Table 6. GA parameters used in these optimization studies have been furnished in Table 7. These results correspond to the problems solved using MATLAB in P–III 500MHz processor personal computer system. The present approach of finding design variables using real coded genetic algorithm 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

Table 6 – *Comparison of RCGA with GRG and NLP – Problem 3*

Design variables unit	Optimal solution		
	GA	NLP	GRG
reactor 1, volume m^3	1182.43	1181.43	1181.4
reactor 2, volume m^3	1248.25	1250.63	1250.6
dryer, volume m^3	891.60	893.31	893.3
pump 1, flow rate m^3 h^{-1}	756.01	753.16	753.1
pump 2, flow rate m^3 h^{-1}	422.93	422.08	422.1
heat Exchanger, flow rate m^3 h^{-1}	422.93	422.08	422.1
pump 3, flow rate m^3 h^{-1}	422.93	422.08	422.1
centrifuge, flow rate m^3 h^{-1}	422.93	422.08	422.1
batch mass capacity, Product 1 kg	891.60	893.31	893.3
batch mass capacity, Product 2 kg	788.29	787.62	787.6
batch mass capacity, Product 3 kg	891.60	893.31	892.9
cycle time, Product 1 h	6.95	6.96	6.963
cycle time, Product 2 h	10.80	10.80	10.799
cycle time, Product 3 h	6.86	6.87	6.865
capital cost $ y^{-1}	159480	159482	159483

Table 7 – *Computational parameters of real coded GA*

RCGA Parameters	Problem 1	Problem 2	Problem 3
Maximum generation	100	500	100
Population size	40	200	50
Number of real coded variables	6	8	14
Selection strategy	roulette	roulette	roulette
Crossover probability	0.9	0.9	0.7
Mutation probability	0.05	0.06	0.05
CPU time, s	1.5	5.0	3.0

solving the complex problem with several variables and nonlinear constraints.

The evolutionary algorithms like GA have been quite successfully applied to a number of difficult optimization problems but the understanding of evolutionary algorithms is as difficult as understanding the natural evolution. These algorithms can be understood intuitively and not with mathematical rigour. The major difficulty in understanding the algorithm is due to the fact it combines two different strategies, a random search by mutation and biased search by recombination of the strings contained in the population. The careful and proper selection of computational parameters enhances the faster convergence, which requires experience and skill in handling these techniques.

Conclusion

This paper demonstrates the successful application of real coded genetic algorithm for the optimal design of reactor network, optimal design of Williams–Otto process plant and multiproduct process plant. It has been found that RCGA can be considered as a complement to the global optimization and conventional techniques. RCGA based optimal design converges faster, does not require complicated mathematical formulations and is efficient in handling problems with large number of discrete variables and constraints. Thus real coded genetic algorithm has proved to be an efficient and effective alternate for the conventional techniques due to its simplicity and ease in implementation for the optimal design of process plants.

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Symbols used

a – Cost coefficient of batch equipment
b – Cost coefficient of continuous equipment
c – Concentration, mol l^{-1}
c – Magnitude of constraint function
F_i – Motor flow rate, mol s^{-1}
q_A – Mass flow rate of fresh feed A, kg s^{-1}
q_B – Mass flow rate of fresh feed B, kg s^{-1}
q_D – Mass flow rate from distillation column bottoms to plant fuel, kg s^{-1}
q_G – Mass flow rate of by product G from reactor and decanter, kg s^{-1}
q_P – Mass flow rate of product P from distillation column, kg s^{-1}
q_R – Total mass flow rate from reactor, kg s^{-1}
q_{RA} – Mass flow rate of A from reactor, kg s^{-1}
q_{RB} – Mass flow rate of B from reactor, kg s^{-1}
q_{RC} – Mass flow rate of C from reactor, kg s^{-1}
q_{RE} – Mass flow rate of E from reactor, kg s^{-1}
q_{RG} – Mass flow rate of G from reactor, kg s^{-1}
q_{RP} – Mass flow rate of product from reactor, kg s^{-1}
f – Capital cost, cost units/year
G – Magnitude of constraint function
k – Reaction rate coefficient, s^{-1}
LVC – Limited violated constraint
M – Molar mass, kg $kmol^{-1}$
P – Port return on investment, %
Q – Volumetric flow rate of continuous equipment, m^3 hr^{-1}
γ – Rate of reaction, kg l^{-1} s^{-1}
S – Batch mass capacity, kg
T – Temperature °C, K
t – Cycle time, h
V – Volume
A – Arrhenius reaction rate pre–exponential factor, h^{-1}
α – Power law coefficient of batch equipment
β – Power law coefficient of continuous equipment
λ – Penalty factor
ρ – Density of the reacting mixture kg m^{-3}
ψ – Objective function
τ – Residence time

Subscripts

i – Batch equipment
j – Continuous equipment

Superscript

S – Steady material balance values

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