Strategies of Multi-Objective Differential Evolution (MODE) for Optimization of Adiabatic Styrene Reactor

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In the present study, two novel strategies of Multi-objective Differential Evolution (MODE) are proposed for solving multi-objective optimization problems. The proposed MODE strategies are applied to ZDT-3 test problem and optimization of industrial adiabatic styrene reactor considering productivity, and selectivity as the main objectives. Four combinations of the objectives are considered for three strategies of MODE algorithms and one set of results are reported here for multi-objective optimization of industrial styrene reactor. Pareto set (a set of equally good solutions) obtained for all the cases is compared with each other for both test problem and industrial styrene reactor optimization problem. MODE-1 is found to have least computational time, whereas MODE-2 algorithm is found to give wide range of results at the cost of computational time.

Keywords: Multi-objective optimization; Differential Evolution; Multi-objective Differential Evolution (MODE); Styrene Reactor; Modeling and Simulation.

1. Introduction

Styrene, $C_6H_5CH{=}CH_2$, is an important monomer used in the manufacture of a variety of plastic products. In terms of monomer production rate, styrene ranks fourth in the United States behind ethylene, vinyl chloride, and propylene [1]. Styrene is produced commercially by catalytic dehydrogenation of ethyl benzene; the average plant capacity is over 100 000 tons per year. Such a high production rate demand for very high operating cost of the plant. In such a case, even a small improvement in the performance of the plant can generate significant revenue.

Significant efforts are devoted by several researchers across the globe during the last two decades in the field of modeling, simulation and optimization of styrene reactor and process. Claugh and Ramirez [2] developed a mathematical model for a styrene pilot plant reactor. They used a steady state version of this model to optimize the location of a steam injection port along the length of catalytic bed. Sheel and Crowe [3] carried out a single objective optimization study of styrene reactor and determined rate coefficients and heat of reactions from the industrial data of an adiabatic styrene reactor using a pseudo homogeneous model. Pseudo homogeneous model have been used by most of researchers for simulation and optimization of industrial reactors [4–7]. Elnashaie et al. [6] developed a rigorous heterogeneous model for the reactor based on dusty gas model for diffusion and reaction in the catalyst pellets. This model was used to extract intrinsic kinetic constants from industrial reactor data iteratively. Clove and Ramirez [2] performed multivariable optimization on both adiabatic and steam injected reactor. Yee et al. [8] used NSGA for multi-objective optimization of industrial styrene reactor. Recently Babu et al. [9] carried out multi-objective optimization of adiabatic styrene reactor using Multi-objective Differential Evolution (MODE). The results were compared with earlier study, and MODE was found to give better results than NSGA mentioned in literature [8]. In the present work, two novel strategies of MODE are proposed for solving multi-objective optimization problems. The developed strategies of MODE are applied to ZDT-3 test problems and optimization of industrial styrene reactor. The results of all the three strategies of MODE are compared.

2. MODE Algorithms

MODE algorithm proposed by Babu et al. [9] has been successfully used for multi-objective optimization of industrial styrene reactor, was found to perform better than NSGA-II. MODE is an extension of Differential Evolution (DE) [10–17] for multi-objective optimization study. Differential evolution is an improved version of Genetic Algorithms (GA) [17]. In the present

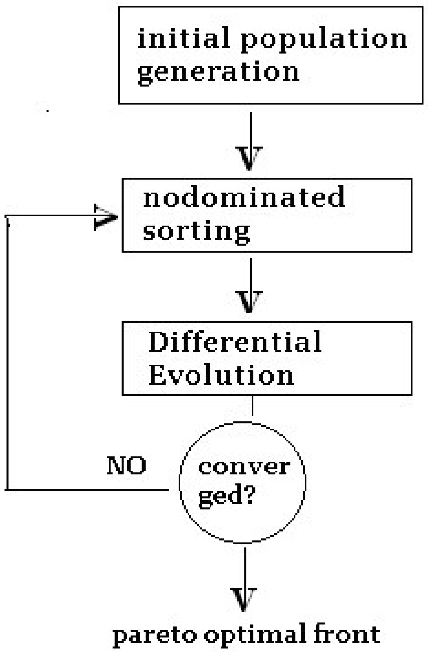

Fig. 1. Simplified flowchart of MODE-1 algorithm.

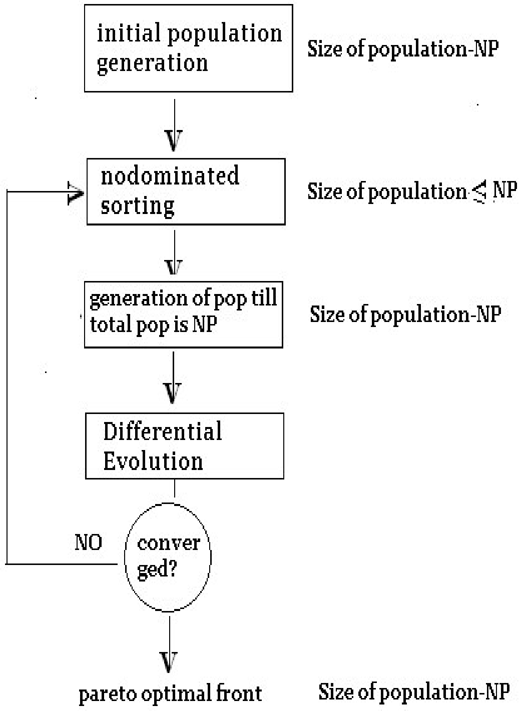

Fig. 2. Simplified flowchart of MODE-2 algorithm.

study two new strategies of MODE algorithm are proposed for solving multi objective optimization problems and their performance is compared with the original MODE algorithm (MODE-1).

2.1. *MODE-1 Algorithm*

The simplified flowchart of the original MODE algorithm (MODE-1) is presented in Fig. 1. The pseudocode for MODE algorithm can be found in literature [9]. In MODE-1 algorithm, in each generation, the dominated solutions are removed from the list and only the non-dominated solutions are allowed to undergo DE operations. The scaling factor is generated from a random number generator between 0 and 1. The off springs are placed into population if they dominate the main parent.

2.2. *MODE-2 Algorithm*

In MODE-1, we are applying non-dominated sorting in each generation. Due to this, the size of population decreases in every generation. In order to perform Differential Evolution operations, we need at least four chromosomes (one target vector and three other vectors for mutation operation). In any generation, if the population size becomes less than four after non-dominated sorting, then it will not be possible to run DE algorithm and Pareto optimal front will not be obtained.

This problem can be overcome by increasing the initial population size. But even then we cannot guarantee that more than four non-dominated solutions will be obtained. Other way is to keep the population size constant in every generation by adding randomly generated chromosomes to the non-dominated chromosomes after non-dominated sorting. As the number of generations increases the non-dominated individuals will increase and finally all the individuals will converge to the Pareto optimal front. Simplified flow chart of MODE-2 is presented in Fig. 2.

The algorithm works as follows: An initial population is generated at random. In every generation all dominated solutions are removed from the population. And same number of random solutions is added to the non-dominated population to maintain the population size constant. DE operations recombination and selection are performed on this population to obtain the next generation individuals. This process continues till stopping criterion is met or Pareto optimal front is obtained.

2.3. *MODE-3 Algorithm*

The recombination operation in DE is proved to be a powerful technique. In recombination, a competition is made between trial and target vectors. It means that there is a competition between the child and Parent vector. The non-dominated vector among the trial and target is sent to the next generations (Survival of the fittest). This domination check alone can give the Pareto optimal front. So the non-dominated sorting before the DE loop can be removed (from original MODE algorithm). At the end of the maximum

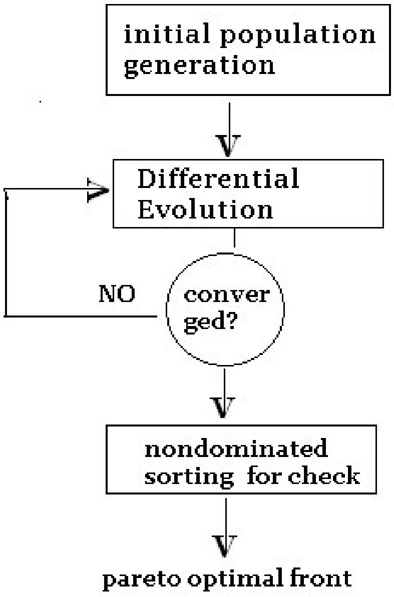

Fig. 3. Simplified flowchart of MODE-3 algorithm.

generations a non-dominated sorting check is kept to remove the individuals which are not on the Pareto optimal front. Same Pareto front and improved solutions are observed when the results of MODE-3 is compared with MODE-1. Simplified flow chart of MODE algorithm 3 is presented in Fig. 3.

The algorithm works as follows: An initial population is generated at random. In every generation DE operations, recombination and selection are performed on the individuals of the population to obtain the next generation of individuals. This process continues till stopping criterion is met or Pareto optimal front is obtained. After the last generation non-dominated sorting is performed to remove the dominated solutions.

3. Objective Function Formulation

3.1. *ZDT-3 Test Problem*

Zitler, Thiele and Deb [18] have constructed six test problems which correspond to non-uniformly represented Pareto- optimal front. We have applied all three MODE algorithms on ZDT-3 problem. ZDT-3 is a 30 variable problem having a number of disconnected Pareto-optimal fronts. The test problem is written as

$$f_1(x) = x_1, \tag{1}$$

$$\mathrm{g(x)} = 1 + \frac{9}{n-1}\sum\nolimits_{i=2}^{n} x_i, \tag{2}$$

$$h\ (f_1, g) = 1 - \sqrt{f_1/g} - (f_1/g)\sin(10\pi f_1). \tag{3}$$

All the 30 variables lie in the range of [0,1].

3.2. *Adiabatic Styrene Reactor*

In this study, maximization of two objectives namely, productivity (F_{ST}) and Selectivity (S_{ST}) are considered. This set of objectives is solved using all three MODE algorithms. The objective functions are as follows

Maximize

$$J_1 = F_{ST} \tag{4}$$

Maximize

$$J_2 = S_{ST} = \frac{F_{ST} - F_{ST}^0}{F_{EB}^0 - F_{EB}} \tag{5}$$

Four decision variables namely, ethyl benzene feed temperature (T_{EB}), pressure (P), steam over reactant ratio (SOR) and initial ethyl benzene flow rate (F_{EB}^0) are considered for optimization. Their bounds are:

$$550 < T_{EB} < 800\,\mathrm{K} \tag{6}$$

$$1 < P < 2.63\ \mathrm{bar} \tag{7}$$

$$7 < SOR < 20 \tag{8}$$

$$27.56 < F_{EB}^0 < 40.56\,\mathrm{kmol/h} \tag{9}$$

Two constraints are also considered for optimization

$$F_{H_2O} < 454\,\mathrm{kmol/h} \tag{10}$$

$$850 < T_1 < 925\,\mathrm{K} \tag{11}$$

Where F_{H2O} an d T_1 are the flow rate of steam and the temperature of ethyl benzene & steam mixture entering the reactor inlet respectively.

The optimization problem considered above is reformulated so as to include the constraints. Penalty function method is employed for handling constraints. The constraints in Eqs. 9 and 10 are incorporated in each of the objectives.

The final from of objective functions considered are as follows

$$I_1 = F_{ST} + 10000\sum_{i=1}^{3} f_i \tag{12}$$

Maximize

$$I_2 = S_{ST} + 10000\sum_{i=1}^{3} f_i \tag{13}$$

Where

$$f_1 = (F_{H_2O} - 454) + |(F_{H_2O} - 454)|, \tag{14}$$

$$f_2 = (850 - T_1) + |(850 - T_1)|, \tag{15}$$

$$f_3 = (T_1 - 925) + |(T_1 - 925)|. \tag{16}$$

The resulting simulation and optimization problems are solved using the proposed MODE algorithms (MODE-1, MODE-2, MODE-3). A subroutine ODE45 (MATLAB Library) was used to integrate all model equations along the length of reactor. The detailed model equations can be accessed from our earlier paper [9]. ODE45 uses IV-order Runge-Kutta method to simulate the model. The model equations for Pseudo-homogeneous model are solved on Pentium IV, 2.4 GHz processor with 256 MB RAM. The computational time for Simulation runs for MODE algorithm 1, 2 and 3 are 6.766 s, 33.7937 s and 24.203 s respectively. The maximum number of generation and size of population considered for study is 10 and 40 respectively.

4. Results and Discussions

4.1. *ZDT-3 Test Problem*

ZDT-3 is 30 variable problem having a number of disconnected Pareto-optimal fronts. All 30 variables lie in the range of 0 and 1. Equations (1)–(3) comprise of the objective functions. The second objective function Eq. (3), h comprise of f_1 (objective 1) in terms of periodic sin function. First objective is in turn a function of x_1. This periodic dependence of first objective function on second objective function give rise to a discontinuous search space. Certain portions of the search space are therefore falls in the dominated region. Figure 4 shows the feasible discontinuous search space for ZDT-3 test problem. The search space is discontinuous in such a way that any multi-objective evolutionary algorithm which does not have an efficient way of maintaining the diversity will have difficulty in giving the well diversified Pareto optimal fronts in all the discontinuous regions. The Pareto optimal region corresponds to $x_i = 2, 3, \ldots 30$, and hence all points satisfying $0 \leq x_1 \leq 1$ lie on the Pareto optimal front. Figure 5 shows the discontinuous Pareto optimal solutions obtained using MODE-1 algorithm. MODE-1 algorithm is applied successfully on multi-objective optimization of adiabatic and pseudo-isothermal styrene reactor. The search space is found to vary between 0 to 1 on X axis (f_1) and -0.75 to 1 on Y axis (f_2). Objective function 2, f_2 contains the *sin* value of objective function 1 (f_1). It is interesting to see that as the value of f_1 increases from 0 to 1, the periodicity is also found to increase. Less amount of discontinuity is observed for lesser value of f_1, whereas as f_1 value increases the discontinuity increases. MODE-1 results (Fig. 5) show that non-dominated solutions are denser for lesser value of f_1. If the value of f_1 is increased, the more number of boundary points of periodic search space, tend to become dominated points. Therefore at higher values of f_1 the Pareto front is less dense.

Figure 6 show the Pareto-optimal solutions for ZDT-3 test problem using MODE-2. We have designed this algorithm in such a way that if the number of non-dominated solutions falls below the predefined value, new chromosomes are produced. These new chromosomes then become eligible partners of the simple evolution strategy of Differential Evolution. In this way, the optimization routine is forced to search the entire search space. This improved version of MODE algorithm is able to find all discontinuous regions with uniform spread of solutions.

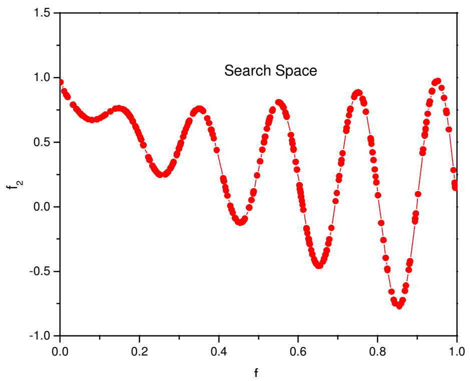

Fig. 4. The Search space for ZDT-3 test problem.

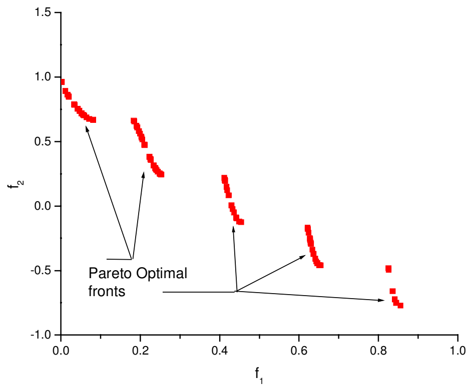

Fig. 5. Pareto front for ZDT-3 test problem using MODE-1 algorithm.

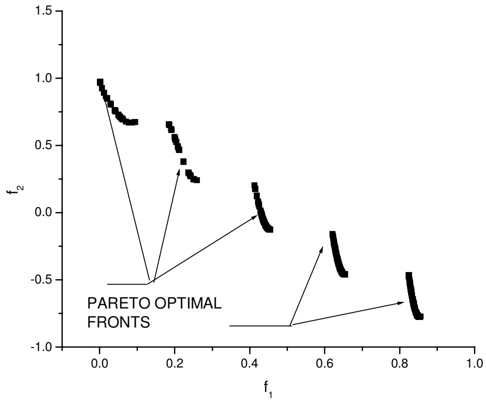

Fig. 6. Pareto front for ZDT-3 test problem using MODE-2 algorithm.

Figure 7 show the discontinuous Pareto-optimal solutions of ZDT-3 test problem using MODE-3. The powerful recombination operation in differential evolution is done by doing crossover between the child and the Parent vector. In this way, there is direct competition between the child and the Parent chromosome. The non-dominated one among those two will survive (by survival of the fittest principle) and will be passed to subsequent generation. Non-dominated sorting is applied only at the end of the algorithm to remove any dominated solutions. The simple and efficient MODE-3 algorithm has given the same Pareto front with comparable spread when compared with the results of MODE-1. MODE-3 also resulted in less uniform spread at higher values of f_1. Comparative Pareto fronts of ZDT-3 test problems for all three proposed algorithms is shown on a single plot in Fig. 8. MODE-2 resulted in uniform spread of solutions, which is evident from Fig. 8.

The percent of points converged to Pareto optimal front is found to be maximum in MODE-2. The design structure of MODE-2 is constructed in such a way that all the population points converge to the Pareto front. The outcome of such algorithm gives the decision maker better flexibility of choosing the solution of his interest from the available solutions. Figure 9 shows that all three proposed algorithms converge to the same Pareto front.

4.2. *Adiabatic Styrene Reactor*

Figure 9 shows the Pareto optimal solutions for adiabatic styrene reactor, discussed in Section 2.2 above. Figure 10 shows the Decision variable T_{EB} plotted against one of the objective function F_{ST}. Styrene is produced by decomposition of ethyl benzene. The decomposition of ethyl benzene to styrene is a reversible endothermic reaction. The endothermic nature of the reactions cause considerable drop in temperature along the length as the reactants flow through the reactor. The yield of styrene drops down along the length of reactor, as higher temperature is favored for the conversion of ethyl benzene to styrene. Constraints Eqs. (10) and (11) are incorporated in the optimization study in order to have the minimum temperature required for reaction to take place (lower bond) and

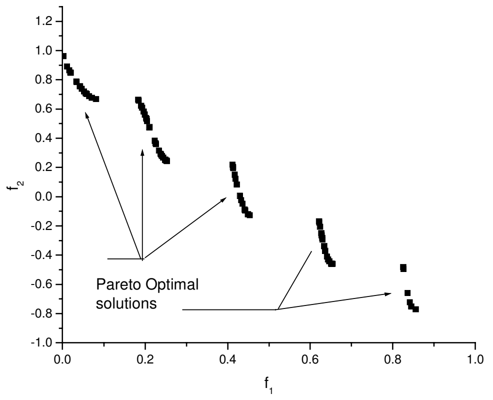

Fig. 7. Pareto front for ZDT3 test problem using MODE-3 algorithm.

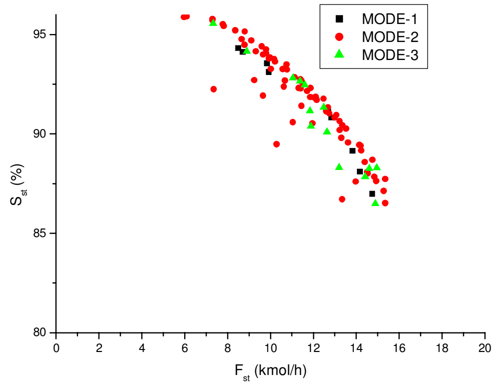

Fig. 9. Comparative Pareto front for Adiabatic styrene reactor using MODE algorithms.

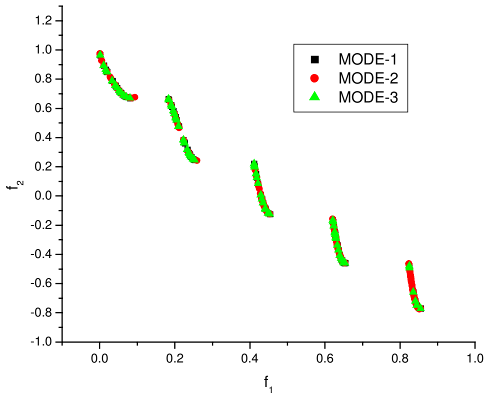

Fig. 8. Comparative Pareto front for ZDT-3 test problem using MODE algorithms.

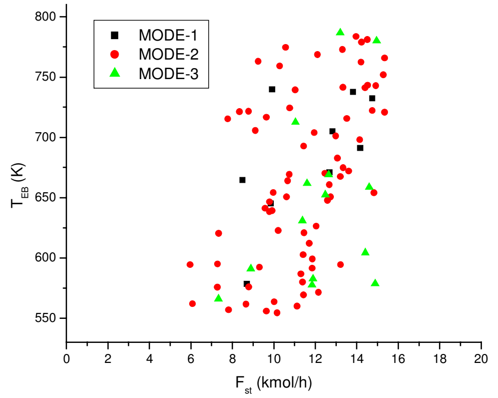

Fig. 10. Decision variable T_{EB} vs. objective function F_{ST} results using MODE algorithms.

to avoid deactivation of catalyst (upper bound of T_1). But as the temperature of reaction mixture increases, side products such as benzene and toluene starts forming. So it becomes extremely important to select the optimum temperature of ethyl benzene at the inlet of reactor.

Figure 10 reveals that styrene productivity is increased with increase in ethyl benzene feed temperature. The upper and lower bound of T_{EB} obtained by all three proposed algorithm in this study is almost same. The optimum temperature of ethyl benzene is found to vary between 550 to 800 K. MODE 2 results give the decision maker an opportunity to choose the solution of his/her interest from the broad range of solution available.

Decision variable P is plotted against F_{ST} in Fig. 11. As the inlet pressure increases the increase in productivity of styrene is observed. The optimum value of pressure is found to vary between 1 bar to 2.6 bar whereas optimum F_{ST} is found to vary between 6 and 16 kmol/h. The points shown in Fig. 10–17 are points corresponding to the Pareto front shown in Fig. 9 for all three algorithms. Figure 12 shows the effect of another decision variable SOR on the productivity of styrene. High SOR gives higher amount of steam per mole of reactant. This leads to increase in feed temperature entering at the entrance of reactor. The higher temperature favors the productivity of styrene. Therefore an increasing trend is observed when decision variable SOR is plotted again F_{ST}. It is interesting to note that even the higher temperature is favored for the productivity, which in turn decreases the styrene selectivity (second objective). The optimum value of SOR did not touch the upper bound. Majority of the optimum decision variable points are found to lie below SOR value of 16, whereas the maximum value of allowable SOR is 21.

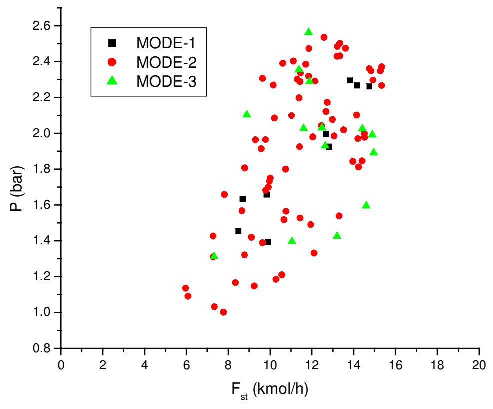

Fig. 11. Decision variable P vs. objective function F_{ST} results using MODE algorithms.

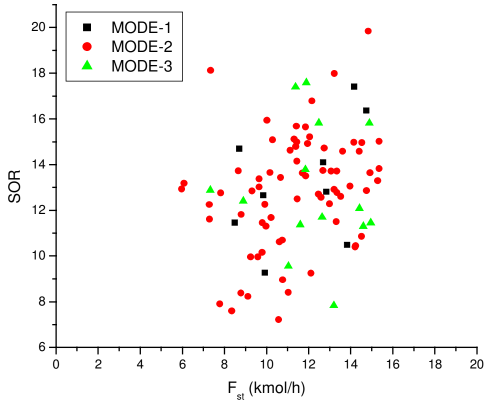

Fig. 12. Decision variable SOR vs. objective function F_{ST} results using MODE algorithms.

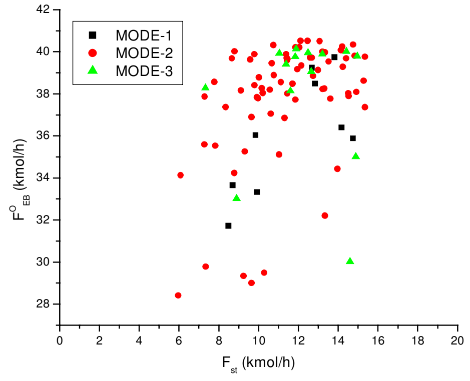

Fig. 13. Decision variable F^0_{EB} vs. objective function F_{ST} results using MODE algorithms.

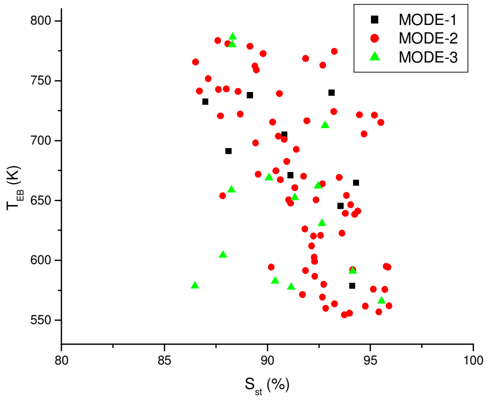

Fig. 14. Decision variable T_{EB} vs. objective function S_{ST} results using MODE algorithms.

Figure 13 shows the optimum values of decision variable F^0_{EB} plotted against one of the objective functions F_{ST}. Initial flow rate of ethyl benzene has significant effect on the reactor performance. Increasing the reactants feed flow rate will give higher productivity. When the two objectives F_{ST} and S_{ST} are considered simultaneously, F^0_{EB} along with TEB and SOR are found to be the controlling variable that resulted in

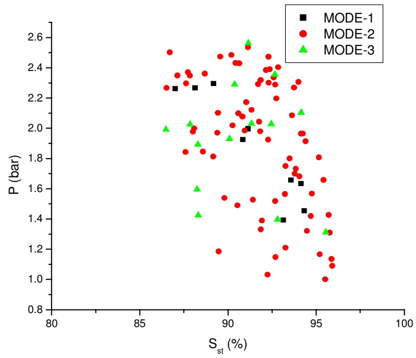

Fig. 15. Decision variable P vs. objective function S_{ST} results using MODE algorithms.

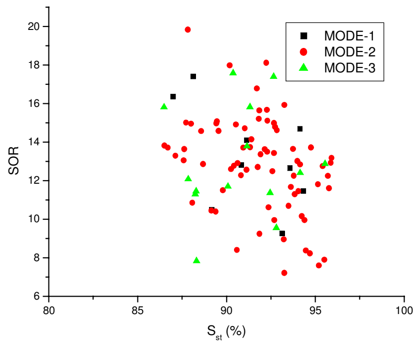

Fig. 16. Decision variable SOR vs. objective function S_{ST} results using MODE algorithms.

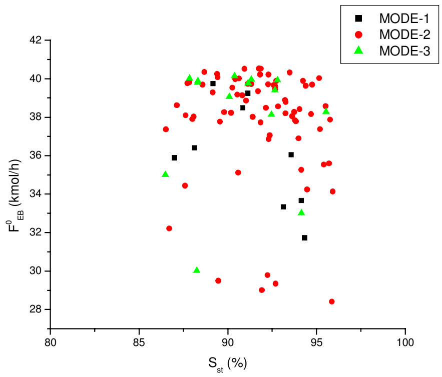

Fig. 17. Decision variable F^0_{EB} vs. objective function S_{ST} results using MODE algorithms.

Pareto optimal front. Majority of the points in Fig. 13 are lying on upper bound of the decision variable. Few chromosomes have F^0_{EB} value less than 34 kmol/h. Value of F_{ST} corresponding to those chromosomes is less than 11 kmol/h. Those chromosomes are part of the Pareto optimal front, due to the conflicting effect of second objective.

Optimum temperature of ethyl benzene feed is plotted against one of the objective functions, S_{ST} in Fig. 14. The decision variable, T_{EB}, vary between the range of 550 to 800 K. As discussed above, a higher temperature is favored for improved productivity. But as the temperature is increased, side products like Benzene and Toluene are produced. Therefore, it needs a compromise while selecting the optimum temperature, when both the productivity and selectivity have to be considered simultaneously. Figure 14 shows that when temperature is increased from lower bound to upper bound, the selectivity decreases from 96% to 87%. The decrease in selectivity of styrene is due to increased temperature, which in turn gives rise to unwanted side products. Majority of the optimum chromosomes in all three algorithms are found to lie in the higher temperature region. (Temperature greater than 650 K). This in turn means that the temperature higher than 650 K is favored for optimum operation of reactor when both the objectives have to be satisfied. The effect of decision variable P on the objective function S_{ST} is shown in Fig. 15. Lower operating pressure is favored optimum operation of the reactor. SOR is found to remain almost between the value of 8 to 16 (see Fig. 16). Also higher selectivity (close to 96%) is observed for SOR value of 8, 11.9, 12.2 and 18. Majority of the points lie in the region of 10 to 16 value of SOR.

The conflicting nature of Pareto front in Fig. 9 is contributed due to the combined effect of decision variables, T_{EB}, SOR and F^0_{EB}. The effect of F^0_{EB} on the selectivity of styrene is shown in Fig. 17. Most of the chromosomes are found to converge towards upper bound of decision variable. Productivity increases at higher feed flow rates. At the same time, when the feed flow rate of ethyl benzene is high, then if it is mixed with steam corresponding to optimum SOR, it will give lesser operating temperature. The Lower operating temperature is favored for increasing the selectivity of styrene. This is evident from Fig. 17.

Table 1 shows the comparative analysis of all the three algorithms (MODE-1, MODE-2, and MODE-3)

Table 1. Comparative % Convergence of Proposed algorithms on different problems.

Problem	Initial Population	Number of Chromosomes converged to Pareto front			% Convergence		
		MODE 1	MODE 2	MODE 3	MODE 1	MODE 2	MODE 3
ZDT-3 Test Problem	300	80	300	80	26.66	100	26.66
Adiabatic Styrene Reactor	40	9	40	14	22.5	100	35

in terms of % convergence. It can be seen that % convergence of MODE-2 is 100%. The % convergence of MODE-1 and MODE-3 is found to be 26.66% for ZDT-3 test problem. The % Convergence of MODE-1 and MODE-3 is 22.5% and 35% respectively on styrene reactor problem.

5. Conclusions

Two Improved versions of MODE strategies (MODE-2 and MODE-3) are proposed in this study. The proposed algorithms are applied successfully on ZDT 3 test problem and on multi-objective optimization of Industrial Styrene reactor and their performance is compared with MODE-1. Pareto optimal solutions are observed for all three proposed algorithms. MODE-2 and MODE-3 algorithms are found to give better solutions than MODE-1 algorithm at the cost of extra computational cost. MODE-2 algorithm has got the advantage of giving maximum possible number of non-dominated solution (equal to size of population). Optimum operating conditions are obtained in terms of temperature of ethyl benzene, pressure, SOR and feed flow rate of ethyl benzene. The decision maker can choose any desired chromosome of his/her interest from the Pareto front. The corresponding decision variables are be accessed during the operation of plant in order to get improved performance of the plant.

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