

Multi-objective Optimization of Styrene Reactor Using Multi-objective Differential Evolution (MODE): Adiabatic vs. Steam Injected Operation

Ashish M Gujrathi^a and B V Babu^{b,*}

^aLecturer, Chemical Engineering Department, Birla Institute of Technology and Science (BITS), Pilani- 333 031, Rajasthan, India. Email:ashishg@bits-pilani.ac.in

^{b*} Assistant Dean -Engineering Services Division (ESD) & Head -Department of Chemical Engineering, Birla Institute of Technology and Science (BITS), Pilani -333 031, Rajasthan, India, Phone: +91-01596-245073 Ext. 205 / 224; Fax: +91-01596-244183; Email: bvbabu@bits-pilani.ac.in, URL: <http://discovery.bits-pilani.ac.in/discipline/chemical/BVb>

ABSTRACT

This paper deals with the multi-objective optimization study for industrial styrene reactor using Multi-Objective Differential Evolution (MODE) algorithm. Two objective optimization study is carried out using objective functions, namely, production, yield and selectivity of styrene for adiabatic as well as steam-injected reactors. Out of the five possible combinations of objectives one combination is reported in this paper. Pareto optimal set (a set of equally good solutions) is obtained for all combinations of objective functions under consideration. The decision variables are plotted against one of the objective functions and results are discussed extensively. Pareto front for both adiabatic and steam-injected reactors is plotted and compared on the same plot. Wide range of optimal solutions is obtained, from which the decision maker can select the one based on the specific requirement in the plant.

Keywords: Multi-Objective Optimization; Multi-Objective Differential Evolution (MODE); Styrene; Pareto Optimal Set; Evolutionary Algorithms; Modeling and Simulation.

INTRODUCTION

Many problems in the process engineering domain tend to deal with a situation that is multi-objective in nature, where more than one objective function needs to be optimized simultaneously. In these situations, the aim is to simultaneously optimize a group of conflicting objectives. Different solutions may produce trade-offs (conflicting scenarios) among different objectives. A solution that is extreme (in a better sense) with respect to one objective requires a compromise in other objectives [1]. In multi-objective optimization, there may not exist a solution that is best with respect to all objectives. Instead, there is a set of equally good solutions called Pareto-optimal solutions. A Pareto optimal set of solution a set of points corresponding to different solution in which when we go from any one point to another in the set, at least one objective function improves and at least one other worsens [2]. Neither of the solutions dominate over each other. All the sets of decision variables on the Pareto front are equally good and is expected to provide flexibility for the decision maker.

Several algorithms are available in the literature [3,4] for solving multi-objective optimization problems e.g. Non Dominated Sorting Genetic Algorithms (NSGA) and its variants, multi-objective genetic local search algorithm, multi-objective simulated annealing, Pareto ant colony optimization. It is observed that classical multi-objective evolutionary algorithms are either not able to give a well diversified and smooth Pareto front or gets converged to a single point solution. However, Evolutionary Algorithms (EA) are expected to find multiple optimal solutions in single run due to their population based search approach. EA's are ideally suited for multi-objective optimization. NSGA, being an EA is expected to give a smooth and well diversified Pareto set. But it found that NSGA gets converged to either a suboptimal solutions or a single point solution. [2] MODE has been successfully applied by our group [10] on adiabatic styrene reactor and obtained a better Pareto front compared to that obtained by NSGA. This is our another attempt to test potential of MODE on multi-objective optimization for adiabatic and steam injected styrene reactors.

Styrene is an important monomer used in the manufacture of a variety of plastic products. It is the raw material for the production of polystyrene, acrylonitrile-butadiene-styrene resins (ABS) and variety of miscellaneous polymers. Several studies on reaction kinetics, reactor modeling, simulation and optimization of styrene reactor have been reported in literature. Clough and

Ramirez [5] 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 part way along the catalytic bed. Sheel and Crowe [6] 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 had been used by most of researchers for simulation and optimization of industrial reactors. [5,7,8,9]. Elnashaie et. al. [7] 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 [5] performed multivariable optimization on both adiabatic and steam injected reactor. Yee et. al. [2] used NSGA for multi-objective optimization of industrial styrene reactor. Recently our group carried out multi-objective optimization of adiabatic styrene reactor using Multi-objective Differential Evolution (MODE) [9]. The results were compared with earlier study, and MODE was found to give better results than the algorithm mentioned in literatures. In the present work, two objective optimization study is carried out using MODE algorithm to obtain Pareto optimal set and optimal operating conditions for both adiabatic and steam injected styrene reactors. The results of this study indicate that there is an improvement in performance when steam is divided into two fractions and injected along the reactor length in addition to reactor inlet.

PROCESS DETAILS AND REACTION SCHEME

Styrene is commercially made from ethyl benzene by direct dehydrogenation of ethyl benzene. Fresh ethyl benzene mixed with recycled ethyl benzene and steam, is preheated using product stream from the reactor and then mixed with the superheated steam to reactor inlet temperature of over 875 K before injecting into fixed bed. Molar ratio of steam to ethyl benzene in feed entering the reactor is usually 15:1. The reactor effluent is cooled to quench all reactions in several heat exchangers and then directed to the separator to recover styrene. The reaction may be carried out either in a series of adiabatic reactors with inter-stage reheating (steam injected) (Fig. 1) or in a pseudo-isothermal operation.

The dehydrogenation of ethyl benzene is endothermic reversible reaction and requires heat input to reach commercially viable conversions. The reaction proceeds with low yield thermally but high yield catalytically. Superheated steam provides necessary heat of reaction inhibits coke formation and reduce the partial pressure of styrene and hydrogen to shift the thermodynamic equilibrium in favor of the styrene production. Six main reactions occurring in the styrene reactor are:

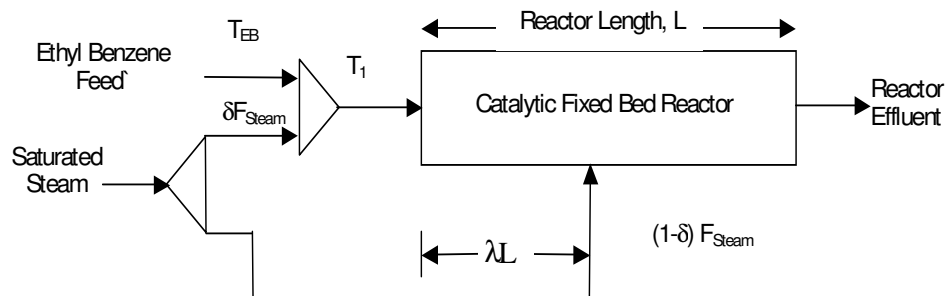
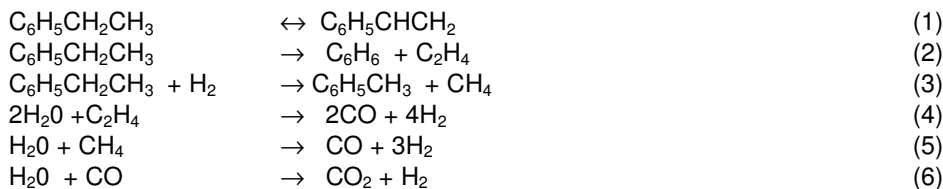


Figure 1. Two bed styrene reactor with steam injection partway of the reactor length.

As this is an endothermic reaction producing two moles of product to one mole of reactant, low pressure and high temperature favor forward reaction producing styrene, $\text{C}_6\text{H}_5\text{CHCH}_2$. At equilibrium, the reversible reaction (Eq. (1)) results in about 80% conversion of ethyl benzene. However, the time and temperature necessary to achieve this give rise to excessive thermal

cracking. The competing thermal reactions (Eqs. (2) and (3)) degrade ethyl benzene to by-products such as benzene (C_6H_6) (Eqs. 2) and toluene ($C_6H_5CH_3$) (Eqs. 3), and thus reduce styrene yield. As the rate of formation of by-products increases with temperature, an optimal operating temperature is necessary to compromise between conversion of ethyl benzene to styrene and by-product formation. In addition, a selective catalyst is desirable to achieve high styrene yield at low temperature and to minimize side reactions.

MULTI-OBJECTIVE OPTIMIZATION OF STYRENE REACTOR REACTOR MODEL

An adiabatic reactor with plug flow and radial uniformity is considered for simulation. For this study pseudo-homogeneous model is used with axial dispersion ignored, and any limitation of mass or transfer the catalyst pellet or diffusion within were lumped into the rate constant. Sheel and Crowe [6] reported the design and operating conditions of this model.

Six equations from material balance, one equation from energy balance, and one from pressure drop suffice to define the model. All kinetic data and model equations are taken from Elnashaie and Elshishini [9], Yee et. al.[2], and Babu et. al. [8]. A subroutine Matlab ODE45 (MATLAB Library) was used to integrate all the model equations along the length of reactor for both adiabatic and steam injected reactor configuration. Several simulation runs were carried out on Intel P4 computer, 3.4 GHz CPU with 1 GB RAM.

OBJECTIVE FUNCTION FORMULATION

In this study, maximization of three objectives namely productivity (F_{ST}), selectivity (S_{ST}) and yield (Y_{ST}) of styrene are considered. The three objectives are

$$\text{Maximize: } J_1 = F_{ST}, \quad (7)$$

$$\text{Maximize: } J_2 = S_{ST} = \frac{F_{ST} - F_{ST}^0}{F_{EB}^0 - F_{EB}}, \quad (8)$$

$$\text{Maximize: } J_3 = Y_{ST} = \frac{F_{ST} - F_{ST}^0}{F_{EB}^0}, \quad (9)$$

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

$$550 < T_{EB} < 800 \text{ K} \quad (10)$$

$$1 < P < 2.63 \text{ bar} \quad (11)$$

$$7 < SOR < 20 \quad (12)$$

$$27.56 < F_{EB}^0 < 40.56 \text{ kmol/h} \quad (13)$$

In the steam injected reactor configuration, a fraction (δ) of steam is mixed with ethyl benzene at the reactor inlet while the remaining steam is injected at a certain point along the reactor, say, at x fraction of the total reactor length. Thus for the adiabatic reactor, δ is equal to 1 and $x(=0)$ is not required. In addition to the above decision variables, two additional variables (δ , fraction of steam used at the reactor inlet and λ , location of injection port of the total reactor length) were used for optimizing steam-injected reactor.

$$0.1 < \delta < 1 \quad (14)$$

$$0.1 < \lambda < 1 \quad (15)$$

Three constraints are also considered for optimization study to accommodate the size limitation of condenser and minimum temperature required for the reaction. The constraint on T_2 is applicable only for steam injected reactor. The constraints are handled by Penalty approach [3]. Those three constraints are

$$F_{STEAM} < 454 \text{ kmol/h} \quad (16)$$

$$850 < T_1 < 925 \text{ K} \quad (17)$$

$$850 < T_2 < 925 \text{ K} \quad (18)$$

RESULTS AND DISCUSSIONS

Maximization of S_{ST} and Y_{ST}

In this case simultaneous maximization of S_{ST} and Y_{ST} (Eqs. 7 and 8) is considered for both adiabatic and steam injected reactor. The set of decision variables with bounds (Eqn. 10 to 13) and constraints (Eqs. 16 to 17) are used for adiabatic operation, while extra decision variables (Eqs. 14 to 15) and the constraint (Eq. 18) is used for the steam injected reactor mode. Fig. 2 shows the Pareto front obtained after 50 generations with 1000 number of population point for case 1 for both adiabatic and steam injected reactor. The trade off among the objective functions can be clearly seen from Fig. 2.

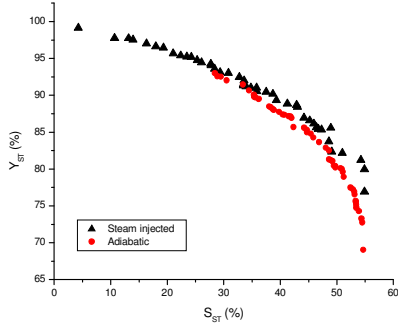


Figure 2. Pareto set for Case 1(S_{ST} Vs. Y_{ST})

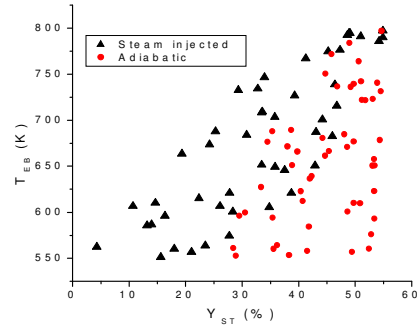


Figure 3. Decision Variable T_{EB} Vs. Y_{ST}

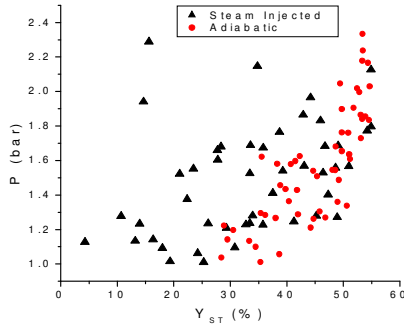


Figure 4. Decision Variable P Vs. Y_{ST}

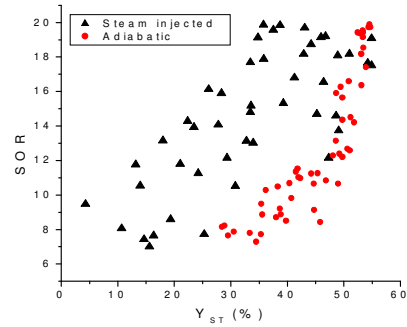


Figure 5. Decision Variable SOR Vs. Y_{ST}

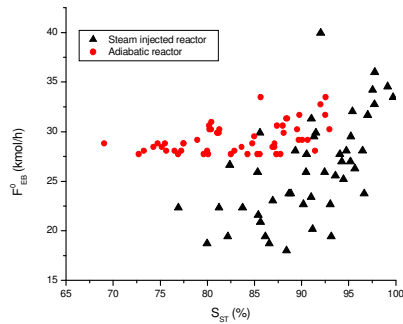


Figure 6. Decision Variable F_{EB}^0 Vs. Y_{ST}

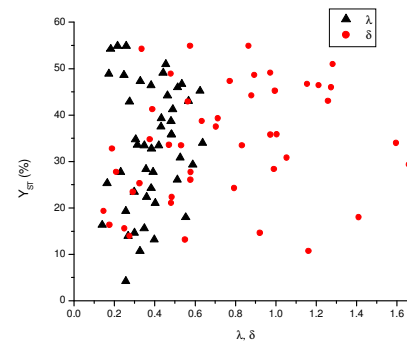


Fig. 7. Delta, Lamda Vs. Y_{ST}

In case of adiabatic operation the minimum value of objective function Y_{ST} is 69.0565 %, the corresponding value of S_{ST} on the Pareto front is 54.7048, which marks the maximum in its entire range of Pareto optimum solutions. The same is true from the maximum value of Y_{ST} (i.e. 92.5575), the corresponding value of S_{ST} on the Pareto front is 28.9102, which is the minimum

value of S_{ST} in the entire Pareto front. The same is true for the case of steam injected reactor operation. This once again confirms the qualitative and quantitative (in terms of number of non-dominated solutions obtained) ability of MODE algorithm for solving Multi-objective optimization problems.

Fig. 2 shows that steam injected operation of reactor gives better Pareto front in terms of both the spread and diversity with respect to both objectives. The preliminary analysis of results clearly shows that the Pareto front obtained by MODE algorithm is better (in terms of spread and diversity) than the one obtained when NSGA was used [2]. Fig. 3 shows the effect of decision variable T_{EB} on objective function Y_{ST} . Fig. 4 and 6 reveals that optimum values of two of the decision variables (P and F_{EB}^0) are nearly constant and that the Pareto front was due to the conflicting nature of the decision variable T_{EB} and SOR. However, the value of decision variable T_{EB} in turn depends on SOR ratio. In the study carried out by Yee et al. it was shown that optimum values of SOR remain constant when plotted against one of the objective functions. But our study shows that yield of styrene increases with SOR in case of adiabatic reactor. But in case of steam injected reactor, this is partially true because of limitation of additional variables, which is discussed below. While dealing with multi-objective optimization of styrene reactor, SOR can be considered as a decision variable (as it controls T_{EB}), which is responsible for the conflicting nature of the Pareto front. It is interesting to note that the highest yield (54.7048 %) is obtained for the T_{EB} value of 796.8705 K, which is the highest value of temperature of ethyl benzene in feed among the optimum decision variables. This means that high temperature of ethyl benzene favors the yield of styrene, while low temperature maximizes the styrene selectivity (S_{ST}). For the lowest available temperature of ethyl benzene the corresponding value of yield and selectivity are 28.9102 % (minimum) and 92.5575 % (maximum) respectively. This is due to the fact that the main reaction (Eq. 1) is a reversible endothermic reaction. Temperature decreases along the length of the reactor, and therefore, high temperature is required to achieve high conversion of ethyl benzene to styrene. This is shown in Fig. 3, where high temperature profile results in higher value of Y_{ST} . However, high temperature promotes thermal cracking leading to a decrease in styrene selectivity, as explained above. Fig. 4 shows the effect of operating inlet pressure on the yield of styrene. It is found that optimum values for decision variable P are nearly constant for both adiabatic and steam injected mode of operation of reactor.

Fig. 5 shows the decision variable SOR plotted against yield of styrene reactor. For both adiabatic and steam injected operation of styrene reactor, it can be seen that yield increases with increase in SOR in adiabatic operation. The point of maximum yield corresponds to the maximum SOR for adiabatic reactor. But the same is not true for the steam-injected reactor. The global optimum or maximum value of yield does not correspond to the maximum SOR. The maximum value of SOR is 19.870923 for which the corresponding yield is 35.7799, while the maximum yield happens to be at the intermediate value of the SOR. The reason for this is again the reversible endothermic nature of the reaction 1 and location of injection port and also the fraction of steam fed at the inlet of reactor. The reason for lower yield even at a higher SOR, is the location of injection port and fraction of steam fed at inlet of steam injected reactor. It is observed that with intermediate SOR value of 17.527599, the yield is maximum, because the value of optimum λ and δ (Fig. 7) for this SOR is 0.2159 (too low or near the inlet of reactor) and 0.5756 (maximum steam almost in the middle of reactor length) respectively. On the other hand, with maximum SOR value of 19.870923, the corresponding optimum yield is 35.7799, as the values of λ and δ for this SOR is 0.4833 (almost half of total steam flow rate) and 0.9732 (at the end of reactor). We wish to highlight this point, because the crux of multi-objective optimization study lies in such conflicting nature of objectives and the decision variables. In fact, process engineers are always in look for such analysis, which may be difficult or even impossible to get from the actual plant operation. This kind of study can help the process and design engineer to either modify the existing design of process plant or can be best suited if consulted with optimization experts before the erection of actual plant in order to maximize the operating profit of plant.

The decision variables F_{EB}^0 is plotted against one of the objectives in Fig. 6. For adiabatic operation, optimum value of initial flow rate of ethyl benzene is almost constant. But again in case of steam injected operation, the nature of optimum decision variable is found to be same F_{EB}^0 is same as that of SOR. Here also the dominant decision variables are the λ and δ .

CONCLUSIONS

Multi-objective differential evolution algorithm is applied successfully on multi-objective optimization of both adiabatic and steam-injected Styrene reactors. Pareto optimal solutions are obtained for the case considered. The Pareto optimal set is found to be smooth and well diversified as compared to earlier studies. The results are discussed qualitatively with reference to process and reaction kinetics. This proves the reliability of MODE algorithm for solving complex multi-objective optimization problems. Few of the limitations of earlier study are also pointed out. The decision variables are plotted against one of the objective function. The results show that the objective functions such as Styrene flow rate, Yield, and Selectivity can be improved by adapting optimal operating conditions. These kind of results are in general valuable to process engineer to study and understand optimal reactor operation. Steam injected operation is found to be better than adiabatic operation.

Notation

F	Molar Flow rate kmol/h
S	Selectivity
SOR	Steam over reactant molar ratio.
T	Temperature, K
Y	Yield
L	Reactor Length

Subscripts

EB	Ethyl benzene
ST	Styrene

Greek letters

δ	Fraction of steam fed at inlet of reactor
λ	Fraction of reactor length.

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