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saurabh Shukla
IIT Delhi, sshukla101@gmail.com

Ankit Anand
Department of chemical engineering, Indian Institute of Technology Delhi, India,
ankitanand1990@gmail.com

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Multi-objective optimization of an industrial styrene reactor using Harmony Search Algorithm

Saurabh Shukla[1], Ankit Anand[2]

Department of chemical engineering,
Indian Institute of Technology
Delhi, India
E-mail: sshukla101@gmail.com[1] , ankitanand1990@gmail.com

Abstract— **Multi-objective optimization of industrial styrene reactor is done using Harmony Search algorithm. Harmony search algorithm is a recently developed meta-heuristic algorithm which is inspired by musical improvisation process aimed towards obtaining the best harmony. Three objective functions – productivity, selectivity and yield are optimized to get best combination of decision variables for styrene reactor. All possible cases of single and multi-objective optimization have been considered. Pareto optimal sets are obtained as a result of the optimization study. Results reveal that optimized solution using harmony search algorithm gives better operating conditions than industrial practice.**

Keywords- Simulation ; Polymer processing ; Styrene ; Multi-objective optimization ; Harmony Search

I. INTRODUCTION

Styrene is one of the most important monomer produced around the world which is used to manufacture polystyrene, acrylonitrile-butadiene-styrene resins (ABS), and a variety of miscellaneous polymers in the petrochemical industry [1-3]. It is fourth most produced monomer after ethylene, vinyl chloride and propylene in US [2]. Styrene is produced commercially by catalytic dehydrogenation of ethyl benzene, and the average plant capacity is over 100000 tons per year. Due to very high scale of production, investment cost is very high and even a minute improvement in the operation can increase profits significantly. Hence, optimal design and operation of the styrene reactor is required.

Many studies on kinetics, reactor modeling, simulation and optimization of the styrene reactor have been reported in the literature. Using pseudo homogeneous model**,** Sheel and Crowe determined the rate constants and heat of reactions by studying the industrial styrene reactor [4]. Claugh and Ramirez 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 [5]. Elnashaie developed a rigorous heterogeneous model based on dusty gas model. They used the model to extract intrinsic kinetic data from industrial data iteratively [6]. Pseudo homogeneous model proposed by Sheel and Crowe is used by most of the researchers for simulation and optimization of industrial styrene reactor.

In recent past many researchers have done optimization study on the styrene reactor with various algorithms. Yee carried out the multi-objective optimization study of styrene reactor for the adiabatic and steam injected reactor operations using non-dominated sorting genetic algorithm (NSGA) [7]. Babu used multi-objective differential evolution (MODE) to carry out multi-objective optimization of adiabatic styrene reactor [8]. The harmony search algorithm, a recently developed meta-heuristic algorithm, is used for multi-objective optimization of adiabatic styrene reactor in this study. The HS algorithm has been successfully applied to various real-world combinatorial optimization problems such as truss structure design, pipe network design; pump switching**,** supply chain management and hydrologic parameter calibration [10-13]**.**

II. HARMONY SEARCH ALGORITM

Harmony Search (HS) algorithm has been developed in an analogy with music improvisation process where musicians in an ensemble continue to polish their pitches in order to obtain better harmony [9].

In the optimization context, each musician corresponds to a decision variable, and the possible notes in the musical instruments correspond to the possible values for the decision variables. The best harmony in music is analogous to the solution vector of optimization, and the musician's improvisations are analogous to local and global search schemes in optimization techniques [14]. Musical performances aims towards finding pleasant harmony (a perfect state) as assessed by an aesthetic standard, just as the optimization process seeks to find a global solution (a perfect state) as determined by an objective function [10].

The parameters of HS method are: the harmony memory size (HMS), the harmony memory considering rate (HMCR), the pitch adjusting rate (PAR), and the number of improvisations (NI). The harmony memory is a memory location where a set of solution vectors for decision variables is stored. The parameters HMCR and PAR are used to improve the solution vector and to increase the diversity of the search process.
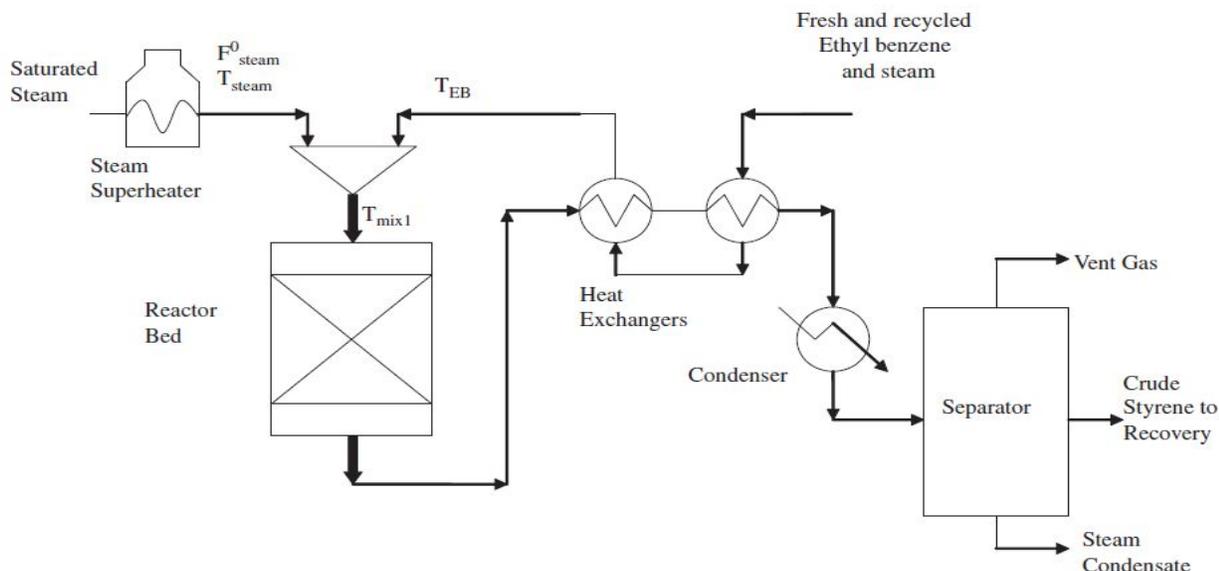
Figure 1: Process flow sheet for production of styrene

Broadly, the HS algorithm consists of the following five steps:

A. Parameter initialization

In the first step, the optimization problem is specified. The HS algorithm parameters are also specified in this step: HMS (harmony memory size= number of simultaneous solution vectors in harmony memory), HMS (harmony memory considering rate), PAR (pitch adjusting rate), and number of improvisations (= number of objective function evaluations).

B. Harmony memory initialization

In this step, Harmony memory is generated with as many randomly generated solution vectors as the size of harmony memory (HMS).

C. New harmony improvisation

Harmony memory vector is improvised with the following three steps –
- Random Selection: As a musician plays any pitch within the instrument range, the value of decision variable is randomly chosen within the value range.
- HM Consideration: the value of decision variable is chosen from any pitches stored in HM with a probability of HMCR (0 < HMCR <1) while it is randomly chosen with a probability of (1-HMCR) in random selection process as previously described.

- Pitch Adjustment: Once one pitch is obtained in HM consideration, a musician can further adjust the pitch to neighboring pitches with a probability of HMCR×PAR (0 <PAR< 1) while the original pitch obtained in HM consideration is just kept with a probability of HMCR × (1-PAR).

D. harmony memory update

If the new Harmony vector is better than the worst harmony in the HM, judged by objective function value, the new harmony is included in the HM and the existing worst harmony is excluded from the HM.

E. termination criterion check

If the termination criterion (number of improvisations) is reached, computation is stopped. Otherwise, Steps C and D are repeated.

Harmony search algorithm is not used extensively in industrial chemical engineering problems. This is the first attempt to apply this novel stochastic algorithm on the industrial styrene reactor.
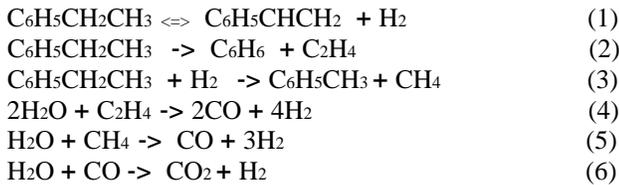
III. ADVANTAGES OF HARMONY SEARCH

Harmony search algorithm is found to have outperformed other stochastic algorithms such as Genetic algorithm, simulated annealing etc. in some recent studies [9,19]. Major advantages of HS algorithm are described below-

- HS makes a new vector after considering all other vectors rather than considering only two (parents) as in Genetic algorithm.
- HS does not require setting up initial values of decision variables.
- HS can solve continuous variable problems as well as combinatorial problems.
- HS converges much faster than other heuristic algorithms. Genetic algorithm [17] and simulated annealing [18] took 250,000 and 70,000 iterations respectively to reach optimal solution in the problem of design of simple network consisting of 7 nodes, 8 links and 2 loops. Harmony Search found same solution after 1095 iterations.[9].
- No complicated calculus such as gradient calculation etc. is involved in HS algorithm. It uses random numbers for its operation.
- Harmony search gives global solution. It does not get stuck in local minima as other deterministic optimization methods.

IV. PROCESS DESCRIPTION

Styrene is made commercially from ethyl benzene by directly dehydrogenating 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. Superheated steam provides the necessary heat of reaction inhibits coke formation and reduces the partial pressure of styrene and hydrogen to shift the thermodynamic equilibrium in favor of the styrene production [7]. Effluent from the reactor is cooled in heat exchangers to stop all the reactions and directed to separation section to recover styrene.

Six main reactions take place in reactor which are given below-

$$C_6H_5CH_2CH_3 \Longleftrightarrow C_6H_5CHCH_2 + H_2 \tag{1}$$
$$C_6H_5CH_2CH_3 \rightarrow C_6H_6 + C_2H_4 \tag{2}$$
$$C_6H_5CH_2CH_3 + H_2 \rightarrow C_6H_5CH_3 + CH_4 \tag{3}$$
$$2H_2O + C_2H_4 \rightarrow 2CO + 4H_2 \tag{4}$$
$$H_2O + CH_4 \rightarrow CO + 3H_2 \tag{5}$$
$$H_2O + CO \rightarrow CO_2 + H_2 \tag{6}$$

Dehydrogenation of ethyl benzene, $C_6H_5CH_2CH_3$ (Eq. (1)) is an endothermic reversible reaction, and proceeds with low yield thermally but with high yield catalytically. As per Le Chatelier's principle, low pressure and high temperature favor forward reaction producing styrene, as it is an endothermic reaction producing two moles of product to one mole of reactant [16]. At equilibrium, conversion of reaction (1) is ~80%. However, high temperature promotes catalytic cracking of ethyl benzene producing unwanted byproducts, benzene and toluene (eq. (2) and (3)). As cracking increases with increasing temperature, an optimal temperature is required to maintain a balance between yield and selectivity.

V. MODEL DESCRIPTION

Sheel and Crowe employed a pseudo-homogeneous model assuming plug flow reactor for simulation of industrial styrene reactor [4]. Heat and mass transfer and diffusion into catalyst pallet were lumped into rate constants. We have used the same pseudo-homogeneous model for our optimization study. Catalyst activity is assumed constant with time and length of the reactor.

The governing equations for the pseudo-homogeneous model, which are used for the multi-objective optimization, are given below [4, 6].

Mass Balance:

$$\frac{dX_i}{dz} = \frac{\rho_b A_t r_i}{F_{eb}^\circ} \tag{7}$$

Where, X_i is the fractional conversion of ethyl benzene in each of the three reactions, i=1, 2 and 3.
For the other three reactions, i=4, 5 and 6, X_i is given by:

$$\frac{dX_i}{dz} = \frac{\rho_b A_t r_i}{F_{steam}^\circ} \tag{8}$$

Energy balance:

$$\frac{dT}{dz} = \frac{\sum_{i=1}^{6}(-\nabla H_i)\,\rho_b A_t r_i}{\sum_j F_j Cp_j} \tag{9}$$

Pressure drop across the reactor length is given by Ergun equation:

$$\frac{dP}{dZ} = 1 \times 10^{-5} \frac{(1-\varepsilon)G_0}{D_p\,\varepsilon^3\,\rho_G}\left[\frac{150(1-\varepsilon)\mu_G}{D_p} + 1.75\,G_0\right] \tag{10}$$

Rate expression and kinetic data for the six reactions are adopted from Sheel and Crowe [4].

VI. MULTI-OBJECTIVE OPTIMIZATION

Multi-objective optimization is done on an existing industrial styrene reactor in which reactor dimensions and catalyst data are already fixed. Three objective functions- productivity, yield and selectivity of styrene produced, are optimized in this study.

Maximize $\quad J_1 = F_{st} \tag{11}$

Maximize $\quad J_2 = S_{st} = (F_{st} - F^0_{st})/(F^0_{eb} - F_{eb}) \tag{12}$

Maximize $\quad J_3 = Y_{st} = (F_{st} - F^0_{st})/(F^0_{eb}) \tag{13}$

For optimizing the operation of an adiabatic reactor, four decision variables are chosen. These and their bounds are:

$850 < T < 925$ K (14)

$1 < P < 2.63$ Bar (15)

$7 < SOR$ (stem to reactant ratio) < 20 (16)

$27.56 < F^0_{eb} < 40.56$ kmol/hr (17)

The constraints on the temperature T of the mixed reactant is based on the minimum temperature required for reaction to take place and the temperature at which catalyst starts to deactivate [5].The range for the inlet pressure, P is chosen based on the pressure at which industrial styrene reactors usually operate. The lower limit of the steam to ethyl benzene molar ratio, SOR (steam over reactant), is set at 7 to prevent coke formation on the catalyst surface and to remove coke deposits from the catalyst surface thereby regenerating it. However, if SOR is increased to a very high value, it will affect the economics of the process as extra energy is required to produce the excess steam and its subsequent condensation at the downstream of the reactor. Hence, it is a usual industrial practice to restrict SOR at 20. The lower and upper bounds for the initial ethyl benzene flow rate, F^0_{eb} are taken to be -25% and +10% of the nominal value (36.87 kmol/h). These bounds are consistent with industrial practice since a plant can often be operated at a much lower capacity but not at a much higher capacity.[7,16]

Harmony search algorithm is mainly used for minimization of objective function without constraints. If an objective function is to be maximized then its reciprocal can be minimized by harmony search algorithm provided it is non-zero at all points. We have used the same strategy for maximization of our objective functions. We have completed our optimization scheme in the following five cases:

Case 1: Individual optimization of productivity (F_{st}), selectivity (S_{st}) and yield (Y_{st}) of styrene.
Case 2: Simultaneous optimization of F_{st} and S_{st}.
Case 3: Simultaneous optimization of F_{st} and Y_{st}.
Case 4: Simultaneous optimization of S_{st} and Y_{st}.
Case 5: Simultaneous optimization of F_{st}, S_{st} and Y_{st}.

With Harmony search, Multi-objective optimization can be done in the following manner-

Minimize:

$$Z = \left|\frac{F_{st-} F^*_{st}}{F^*_{st}}\right| + \left|\frac{S_{st-} S^*_{st}}{S^*_{st}}\right| \quad (18)$$

As seen in the above equation, the multi-objective function is expressed as the sum of the absolute values of relative errors between optimal value and current function value, where the optimal value for each objective function can be calculated beforehand using single objective functions for productivity and selectivity, respectively. F^*_{st}, Y^*_{st} and S^*_{st} are the optimal vales of productivity and selectivity respectively which are obtained by single objective optimization of both functions. Pareto front for two objective optimization can be obtained by minimizing the function below with different sets of values of a and b –

$$Z = a \left|\frac{F_{st-} F^*_{st}}{F^*_{st}}\right| + b \left|\frac{S_{st-} S^*_{st}}{S^*_{st}}\right| \quad (19)$$

In our case, range of a and b values is [1, 7].

Similarly, for three-objective optimization, the following error function is minimized –

$$Z = \left|\frac{F_{st-} F^*_{st}}{F^*_{st}}\right| + \left|\frac{S_{st-} S^*_{st}}{S^*_{st}}\right| + \left|\frac{Y_{st-} Y^*_{st}}{Y^*_{st}}\right| \quad (20)$$

VII. RESULTS AND DISCUSSION

Pseudo- homogeneous model of reactions is used in this study. All the data has been adopted from literature [6,7,8,15,16]. Six mass balance, one energy balance and one momentum balance equation have been simultaneously solved to compute conversion of the reactants.

Styrene reactor model is optimized by harmony search algorithm on computer with core2duo processor and 4 GB RAM. Model equations were solved using inbuilt subroutine ODE45 of MATLAB software.

Harmony search parameters used in this study are given in Table 1.

TABLE 1: Harmony search parameters used in the study-

S. No.	Parameter	Value
1	Harmony memory size(HMS)	10
2	Harmony memory considering rate(HMCR)	0.8
3	Pitch adjusting rate(PAR)	0.4
4	Number of improvisations	1000

A. Single objective optimization

Results of single objective optimization study are shown in Table 2. Maximum obtained selectivity is 96.36% while Maximum yield obtained is 44.36%. Maximum productivity of 16.13 kmol/hr is also obtained. Since dehydrogenation

reaction is endothermic, maximum yield and productivity are obtained at maximum allowable temperature (925 K). At higher temperature thermal cracking increase and undesirable products e.g. benzene and toluene are produced in greater quantities. Selectivity decrease as we increase temperature. Hence, maximum selectivity is obtained at minimum temperature (850 K).

TABLE 2   Objective function and decision variables obtained in single objective optimization

S. No.	Objective function	Value of objective function	P (Bar)	T (K)	SOR	F^0_{eb} (kmol/h)
1	Productivity (kmol/hr)	16.13	2.63	925	13.412	40.56
2	Selectivity (%)	96.36	1	850	15.76	40.37
3	Yield (%)	44.36	2.63	925	18.03	27.56

Along the length of the reactor temperature and pressure both decrease. For the case when conversion is at the maximum value, temperature and pressure profiles are shown in Fig. 2 and Fig. 3.
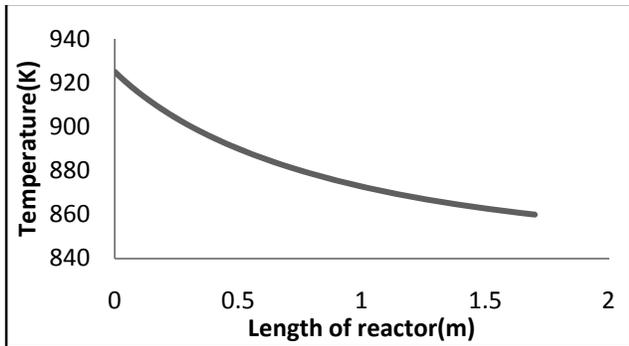

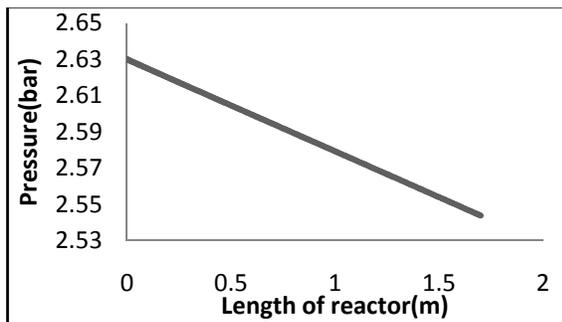Figure 2: Temperature profile along the length of the styrene reactor.

Figure 3: Pressure profile along the length of the styrene reactor.

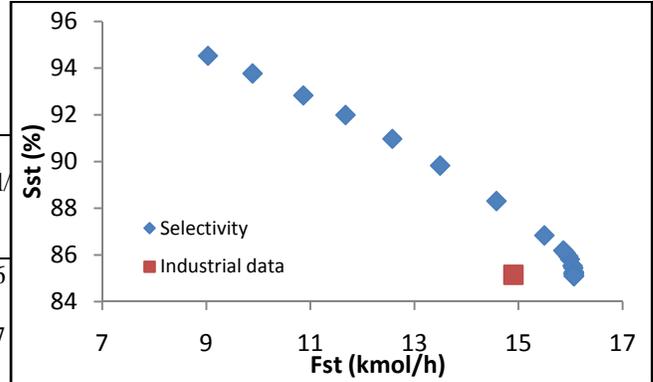B. *Two objective optimization of F_{st} and S_{st}*

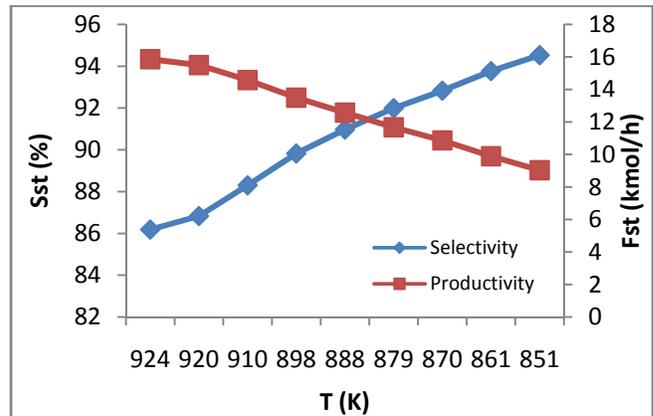Figure 4: Pareto front obtained by two-objective optimization of F_{st} and S_{st}

Figure 5: Selectivity and Productivity as a function of decision variable T

Fig. 4 shows the Pareto optimal set obtained for two objective optimization of F_{st} and S_{st}. Each point on the Pareto set corresponds to a set of decision variables (T, P, SOR and F^0_{eb}). Results show that the optimum values for three of the decision variables (P, SOR and F^0_{eb}) are nearly constant and that the Pareto generated is primarily due to contribution of the decision variable, T. High T maximizes styrene produced (F_{st}) while low T maximizes styrene selectivity (S_{st}) (Figure 5). This is due to the fact that the main reaction (Eq. (1)) is a reversible endothermic reaction. However, high temperature promotes thermal cracking leading to decrease in the styrene selectivity. The optimal results also show that the decision variable, F^0_{eb}, hits the upper bound as it is obvious from the fact that high reactant flow rate will produce more styrene.

C. Two objective optimization of S_{st} and Y_{st}

In this case Y_{st} and S_{st} are optimized simultaneously. Pareto front obtained for this case is shown on Fig. 6. It can be noted that Pareto front consists of the optimized points which show better performance than the industrial operating point.
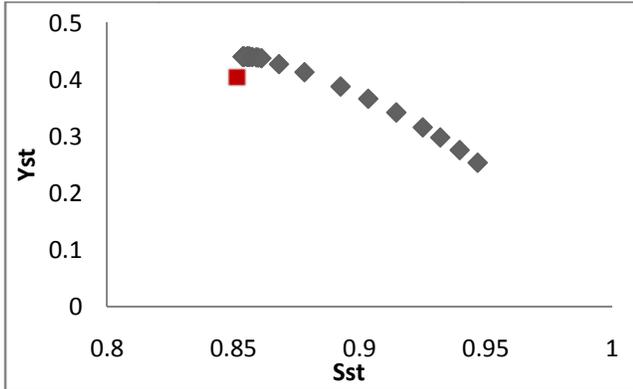

Figure 6: Pareto front obtained by two objective optimization of Y_{st} and S_{st}.

As selectivity increases, yield of styrene decreases. Temperature and pressure has a proportional effect on yield and inverse effect on selectivity. F^0_{eb} is around 14 kmol/hr (lower limit) for every point on Pareto set. Reason behind this observation is that lower value of F^0_{eb} maximizes the yield and does not affect selectivity much.

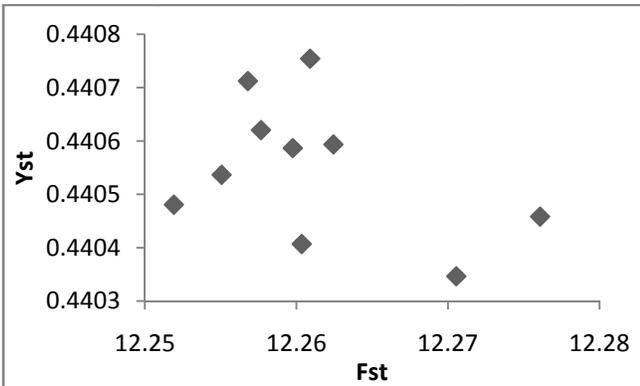## D. Two objective optimization of F_{st} and Y_{st}

Figure 7:Pareto front obtained by two objective optimization of F_{st} and Y_{st}.

In this case temperature remains constantly at its upper bound since high temperature favors both productivity and yield. Pressure also remains constant at each optimized point. F^0_{eb} and SOR are the controlling variables for this case and vary in the set of solutions. High F^0_{eb} promotes high productivity and low yield. Due to the conflicting effect of F_{st} on each objective function, we get randomly scattered optimized solutions (Fig. 7). Any of the optimized can be selected on the basis of rational decision of operator.

E. Three objective optimization

Table 3 shows the unique set of decision variables obtained from three objective optimization of F_{st}, S_{st} and Y_{st}. A cumulative error function was formed, for each of the objective functions, which was minimized using Harmony search algorithm. Table 3 also shows comparison with the industrial data. It must be noted that F_{st} obtained from three objective optimization using Harmony search is greater than F_{st} from industrial data. S_{st} and Y_{st} can be considered practically same for both the cases.

TABLE 3: Results of three-objective optimization

Parameter	This study(HS)	Industrial data
Productivity (F_{st})	16.0468733 kmol/hr	14.90 kmol/hr
Selectivity (S_{st})	85.445 %	85.15%
Yield (Y_{st})	39.58%	40.30%

VIII. Conclusions

Harmony search algorithm is used to simulate and optimize the industrial adiabatic reactor. Four decision variables are used to perform single and multi objective optimization. Pareto optimal sets were obtained for all two objective optimization cases considered. Unique sets of decision variables were also obtained for all single objective cases and three-objective optimization. The trends of decision variables obtained with respect to the objective functions are explained qualitatively and quantitatively for all the cases under consideration. The combination of optimum decision variables obtained using Harmony search algorithm found to give better results in terms of productivity, yield and selectivity when compared to the existing operating conditions in the industry. The Pareto optimal set obtained for two objective optimization of F_{st} and Y_{st} gave randomly scattered sets of optimal solutions. Hence, no definite trend was observed as obtained from the other two-objective optimization cases. In the field of industrial chemical engineering, there are few studies where Harmony search algorithm has been employed to solve optimization problems. Thus this study introduces the application of Harmony search for solving complex industrial optimization problems. It has also been shown that the recently developed Harmony Search algorithm works effectively for multi-objective optimization problems.

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