

Multi-objective Genetic Optimization of Ethane Thermal Cracking Reactor

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Abstract

An industrial ethane thermal cracking reactor was modeled assuming a molecular mechanism for the reaction kinetics coupled with material, energy, and momentum balances of the reactant-product flow along the reactor. To carry out the multi-objective optimization for two objectives such as conversion and ethylene selectivity, the elitist non-dominated sorting genetic algorithm was used. The Pareto optimum set was obtained successfully and finally the effect of the decision variable was discussed.

Keywords: Optimization, Genetic algorithm, Thermal cracking, Ethane

1- Introduction

Thermal cracking of light hydrocarbons such as ethane, propane, n-Butane, i-Butane and their mixtures are the main processes for the production of olefins. Hydrocarbon feed stock mixed with the process steam are introduced into tubular reactors (cracking coils) with short residence times and high temperatures. The process steam is basically an inert gas that serves the purpose of increasing olefin selectivity and reduces coke formation by reducing the hydrocarbon partial pressure. The paraffin feed stock is thermally cracked into mainly olefins, aromatics, methane and hydrogen. The homogeneous cracking reactions are endothermic and need energy input in order to reach gas temperatures as high as 800 -900°C at the coil outlet.

The heat required for endothermic reactions

is provided via radiation burners in the sidewall or long flame burners in the bottom of the furnace. Thus, several cracking coils are placed vertically inside a fire box and heated with hydrogen/methane fueled burners. The reactions are quenched in the transfer line exchanger (TLX) and steam is generated. Steam is superheated and feed stock and process steam are preheated with the flue gas in the convection section of the furnace [1]. Ethylene monomer is one of the base petrochemicals that form the building blocks of the petrochemical industry and is produced in the largest volume among them. The bulk of ethylene produced is used in the production of plastics, primarily polyethylene. Moreover, it is an ideal base material for many other petrochemicals, as it is readily available at low cost and high purity, and usually reacts with other low cost

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materials such as oxygen and water. Therefore, it can be perceived that even a small improvement in the processing of ethylene has the potential of bringing a high dividend to the petrochemical industry.

There are several reports on the optimization of thermal cracking plants. Optimal operation of ethylene plants at variable feed conditions has been reported by Eliceche et al [2-3]. Dynamic optimization of the production period of thermal cracking has been used with respect to coke formation in cracking coil and TLX. The standard SQP package has solved the optimization problem [4]. Shahrokhi et al reported the simulation and optimization of naphtha thermal cracking in a pilot plant [5]. In another work, optimal temperature profile has been used in the control of propane thermal cracking [6]. Lim et al developed the optimal decoking scheduling strategies for the industrial naphtha cracking furnace system. The problem has been formulated as an MINLP [7]. In this work the elitist nondominated sorting genetic algorithm (NSGA-II) is used for the optimization of the thermal cracking of ethane. Simultaneous maximization of two objective functions such as ethane conversion and ethylene selectivity are carried out using NSGA-II.

2- Elitist non-dominated sorting genetic algorithm

Most chemical engineering problems require the optimization of several objective functions, and hence, require the use of multiobjective optimization techniques. Traditionally, multiobjective functions are reduced to a single objective function by various methods and then solved as a single objective optimization technique. All of these methods depend on the user's decision to specify weights to the different objective functions, and are therefore highly dependent on the judgment of the user. Thus the user must have good knowledge on fixing the priority for the different objective functions

to form a single objective function from multiple objective functions. The user may change the priorities and solve the problem to get a number of solutions. The set of all the solutions is known as the Pareto optimal set. But the Pareto optimal set cannot be obtained simultaneously in a single run. Genetic algorithm has the advantage of obtaining the Pareto optimal set in a single run [8].

NSGA-II starts with a population of random solution (Npop). In the Nth iteration the offspring population is first created by using the parent population and the usual genetic operators—reproduction, recombination and mutation. Thereafter, both populations are combined together to form a new population of size 2Npop. A non-dominated sorting procedure is then applied to classify the entire population into a number of hierarchical non-dominated fronts. In the final stage, the final population with the size of Npop is selected using crowding distance sorting and the next generation is started [9].

In recent years multi-objective genetic optimization has been used in many areas of chemical engineering. Rajesh et al have used non dominated sorting genetic algorithm (NSGA) to maximize the export steam and hydrogen production rate in a hydrogen production plant using steam reforming of methane by optimizing gas temperature, pressure and composition in a steam reformer, as well as the temperature of the high temperature and low temperature shift converters [10]. Silva and Biscaia have used GA to obtain a Pareto optimal set of temperature and initiator feed so as to maximize the monomer conversion and minimize the residual initiator concentration for a bath styrene polymerization process [11]. Application of NSGA in reaction engineering has been reviewed by Nandasana et al [12].

Multiobjective evolutionary computation has been used in the epoxy polymerization process, and the combination of minimization or maximization of objectives,

such as the number average molecular weight, polydispersity index and reaction time has been considered [9]. Bhutani et al have reported multiobjective optimization of an industrial hydrocracking unit. The NSGA-II has been used for simultaneous maximization and minimization of two objective functions using eight decision variables [13]. In another work, optimization of an industrial low density polyethylene tubular reactor has been carried out using NSGA-II. The simultaneous maximization of monomer conversion and the minimization of normalized side product has been considered for optimization [14]. Sankararao and Gupta [15] have reported multiobjective optimization of pressure swing adsorbers (PSA) for air separation. The optimization process was used for two two-objective problems and a four objective function problem in the operation of PSA.

3- Model formulation and sensitivity analysis

A multiobjective optimization study with NSGA-II requires execution of the thermal cracker model for each member of its population over a certain number of generations. Because the number of population typically ranges from 50 to 100 and the number of generations needed to find a reasonably good Pareto can be more than 200, a typical study involves computation of the steam cracker model 10,000-20,000 times. Such a huge computational load makes the molecular mechanism of cracking reactions look more attractive, as it results in nonstiff differential equations and hence requires lower computational times, although it's obtained in a tradeoff with prediction accuracy. In this study the molecular mechanism which involves with 7 of reaction and 8 molecular species was considered. The reaction mechanism proposed by Froment et al assumed that reactions are elementary, and therefore, the order of each reaction corresponds to molecularity.

The set of used continuity equations for the various process gas species including the energy and momentum equations were as follows:

Mass balance:

$$\frac{dF_j}{dz} = \left(\sum_i s_{ij} r_i \right) \frac{\pi d_t^2}{4} \quad (1)$$

Energy balance:

$$\sum_j F_j C_{pj} \frac{dT}{dz} = Q(z) \pi d_t + \frac{\pi d_t^2}{4} \sum_i r_i (-\Delta H)_i \quad (2)$$

Momentum balance:

$$\left(\frac{1}{M_m P_t} - \frac{P_t}{\eta \cdot G^2 RT} \right) \frac{dP_t}{dz} = \frac{d}{dz} \left(\frac{1}{M_m} \right) + \frac{1}{M_m} \left(\frac{1}{T} \frac{dT}{dz} + F_r \right) \quad (3)$$

with the friction factor:

$$F_r = 0.092 \frac{Re^{-0.2}}{d_t} + \frac{\zeta}{\pi R_b} \quad (4)$$

and for the tube bends as:

$$\zeta = \left(0.7 + 0.35 \frac{\Lambda}{90^\circ} \right) \left(0.051 + 0.19 \frac{d_t}{R_b} \right) \quad (5)$$

A detailed description of the applied mathematical model can be seen elsewhere in [16].

A sensitivity analysis was performed with the mathematical model to note the effects of some key variables identified as the decision

variables in the subsequent optimization study on the reactor performance. The variables are the temperature (T_{in}) and pressure (P_{in}) of the ethane-steam mixture at the inlet to the radiation section; the steam-to ethane (mass) ratio (SR); and the ethane flow rate (F_{in}) to the reactor. The values of each of these variables were varied within a preassigned domain, while the others were kept constant, to note the effects of variation on some calculated quantities that show the reactor performance. These quantities are the conversion (X) of ethane, and the selectivity of ethylene (Sc_2H_4), which together defines the extent and the quality of the reaction process.

Furthermore, the three additional variables such as residence time, average reaction temperature, and average reaction pressure were calculated along with the performance variables to develop a clearer understanding of the effects of the decision variables. These three variables were calculated in the following way:

$$t_r = \int_0^L \frac{\left(\frac{\pi}{4} d_{in}^2\right) dx}{\left[F_{steam}(x) + \sum_j F_j(x) \right] \frac{RT(x)}{P(x)}} \quad (6)$$

$$T_{av} = \frac{\int_0^L T(x) dx}{L} \quad (7)$$

$$P_{av} = \frac{\int_0^L P(x) dx}{L} \quad (8)$$

The range of each decision variable was as follows: Inlet temperature (700-900K), inlet pressure (290-500kPa), steam ratio (0.25-0.5)

and inlet feed rate (0.019-0.025 kmol/s). The outcome of the entire analysis is presented in Figure. 1.

The sensitivity analysis of the inlet temperature shows that an increase in temperature resulted in increased ethane conversion and decreased ethylene selectivity (Figure1). The main reason behind the sharp conversion increment is the increase in average reaction temperature and decrease in average pressure. Low residence time and low pressure improve selectivity, but in the present case, the influence of the high reaction temperature, which reduces selectivity, had a more dominant effect. On the other hand, the effect of reaction pressure on the cracker performance is not very substantial. An increase in pressure increased the ethane conversion while decreasing the ethylene selectivity. An increase in pressure most prominently influenced the residence time, as can be seen in Figure 1. It seems that high residence time and high reaction pressure had a contradictory effect on the reaction.

Steam reduces the reaction pressure in two ways: by acting as a diluent, it decreases the partial pressures of the reactants, and by increasing the overall flow rate through the reactor, it increases the total pressure drop as well. Consequently, as the SR increased, the conversion decreased and the selectivity increased. The net residence time decreased as the net flow rate through the reactor increased and the reactor dimensions remained the same. Decreases in the residence time and the reaction pressure counteracted each other and resulted in little or insignificant variation of the conversion.

Increasing the ethane feed rate sharply decreased the conversion while increasing the selectivity. The main reason for the former is the sharp decrease in residence time as flow rate increased. The rise in selectivity resulted from the decreased reaction temperature, reaction pressure, and residence time.

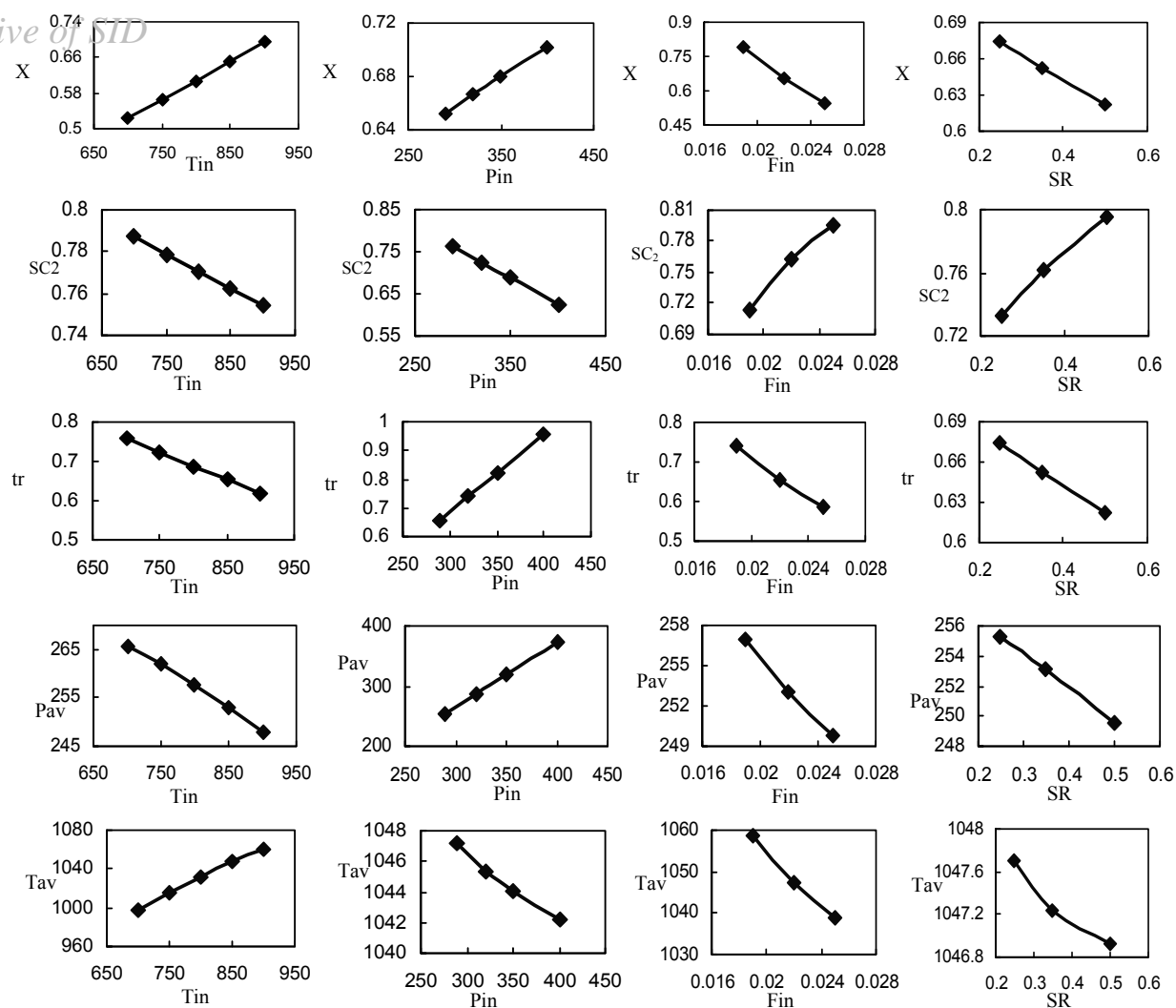


Figure 1. Sensitivity of ethane conversion, ethylene selectivity, residence time, average temperature and average pressure in the reactor to decision variables.

4. Optimization problem

From the reaction point of view, the most pertinent objectives are to maximize the ethylene production and minimize the production of side products. Therefore, the conversion of ethane and selectivity of ethylene were chosen as the objectives. In the sensitivity analysis section, it was observed that the conversion and selectivity vary in opposite directions. Hence, the conversion of ethane and selectivity of ethylene were chosen as the objectives so that a nondominated set of solutions could be obtained from a multiobjective optimization.

Accordingly, the optimization problem was formulated to maximize conversion and selectivity simultaneously. But NSGA-II is based on minimization of the problem. Therefore, the maximization problem was transformed to a minimization one as follows:

$$J_1 = \frac{I}{(X + I)} \quad (9)$$

$$J_2 = \frac{I}{(S_{C_2} + I)} \quad (10)$$

As with many optimization methods, NSGA-II requires a set of operators to carry out the optimization. In this study the simulated binary crossover (SBX) and polynomial mutation were used for creating a new population. Deb [17] has developed these operators for real GA. The following steps were used for its implementation:

- i) Generate random number $u_i \in [0,1)$ for each gene in a chromosome.
- ii) Calculate spread factor as shown below:

$$\beta_{qi} = \begin{cases} (2u_i)^{\frac{1}{1+\eta_c}} & \text{if } u_i \leq 0.5 \\ \left(\frac{1}{2(1-u_i)}\right)^{\frac{1}{1+\eta_c}} & \text{otherwise} \end{cases} \quad (11)$$

- iii) β_{qi} is then used to find the offspring as follows:

$$\begin{aligned} x_i^{(1,t+1)} &= 0.5[(1 + \beta_{qi})x_i^{(1,t)} + (1 - \beta_{qi})x_i^{(2,t)}] \\ x_i^{(2,t+1)} &= 0.5[(1 - \beta_{qi})x_i^{(1,t)} + (1 + \beta_{qi})x_i^{(2,t)}] \end{aligned} \quad (12)$$

Where, t denote the generation number. The polynomial mutation is a polynomial function similar to that of the SBX operator. The mutated gene of a string is found to be:

$$y_i^{(1,t+1)} = x_i^{(1,t+1)} + (x_i^U - x_i^L)\bar{\delta}_i \quad (13)$$

Where the parameter $\bar{\delta}_i$ is calculated using the equations below:

$$\bar{\delta}_i = \begin{cases} (2r_i)^{1/(\eta_m+1)} - 1 & \text{if } r_i < 0.5 \\ 1 - [2(1-r_i)]^{1/(\eta_m+1)} & \text{if } r_i \geq 0.5 \end{cases} \quad (14)$$

A detailed description of these operators and NSGA-II algorithm are available in [18].

5- Constraints handling

Constraints, in general, are the integral part of most of the real world optimization problems. Most applications use an external penalty term, which penalizes infeasible solutions. Many classes of constraints handling methods for gas exist [12]. In this study the distance based static penalty method was used for constraint handing. The optimization is subject to the following constraints:

$$\begin{aligned} T &\leq 1300 \text{ K} \\ P_{out} &\geq 120 \text{ kPa} \end{aligned} \quad (15)$$

where T and P_{out} are reaction temperature and outlet pressure. The upper limit of the reaction temperature is bound by metallurgy of the radiant coil. If the temperature exceeds 1300 K, the coil can rupture so the upper limit of the temperature at any point along the reactor length was fixed at 1300 K. The outlet pressure constraint was gained by the suction pressure of the cracked gas compressor.

All of the computations were performed on a personal computer with a Dual Core AMD Athlon 64 X2, 3016 MHz (15 x 201) 6000 processor and 2G of SDRAM. The average CUP time taken for each study was 8 min.

6- Results and discussion

The primary outcome of multiobjective optimization is the Pareto optimal set of solutions depicting tradeoffs between the competing objectives. In addition, values of the decision variable and the trends of variation of these variables with respect to the objectives are important as well. In the following sections the Pareto set that was obtained in optimization is depicted, and further studies were carried out on tuning of NSGA-II parameters.

6.1 - Simultaneous maximization of ethane conversion and ethylene selectivity

The Pareto-optimal set obtained by maximizing the ethane conversion and the ethylene selectivity is presented in Figure 2, which shows that the Pareto set generated by NSGA-II was smooth and well distributed over a wide range. Of the solutions in the initial population, some were infeasible, but the constrained nondominated sorting method brought the entire population into the feasible region by few generations.

Figure 2 shows only the feasible solutions of the initial population. It can be noted that the feasible solutions are not far from the final Pareto set, from the initial population itself. This is because of the starkly contradictory nature of the objectives, for which simultaneous decreasing of both objectives is not possible below a certain limit. This limit,

the Pareto of simultaneous minimization of selectivity and conversion, is also presented in Figure 2.

6.2 - Effect of NSGA-II parameters on Pareto front

The Pareto presented in Figure 2 was the best obtained from experimentation with different combinations of NSGA-II parameters. Figure 3 shows the effect of the number of generations on the Pareto front. It can be seen that by increasing this parameter the Pareto front can be improved, but when the number of generations is set on 400 generations, it is obvious that a minor change has taken place in the Pareto front, and furthermore, it can take more CUP time. Therefore, 200 generations was selected for further studies.

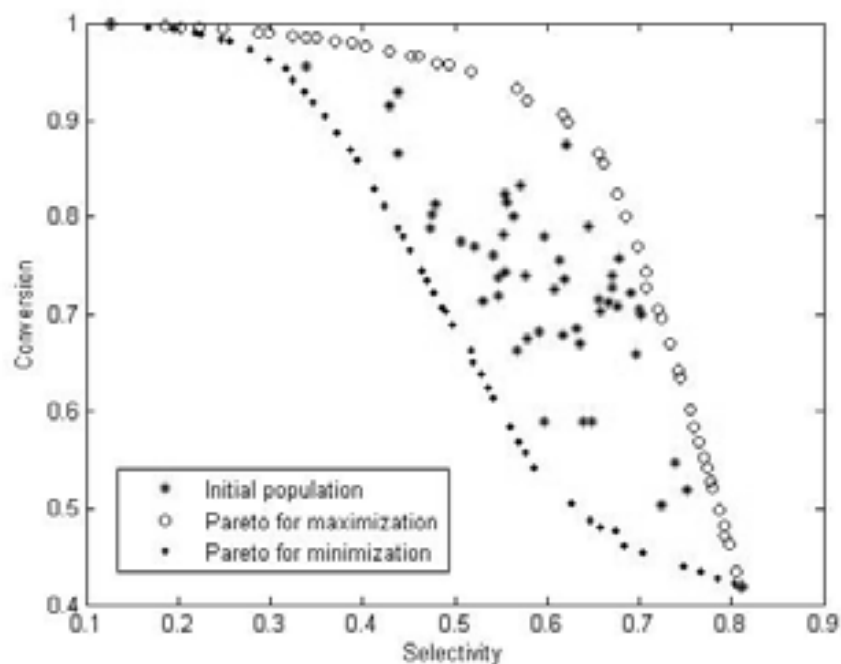


Figure 2. Pareto set obtained for the simultaneous maximization and minimization of ethylene selectivity and ethane conversion. Also, feasible points of initial population are plotted. $\eta_c = \eta_m = 0.01$, $N_{pop}=50$.

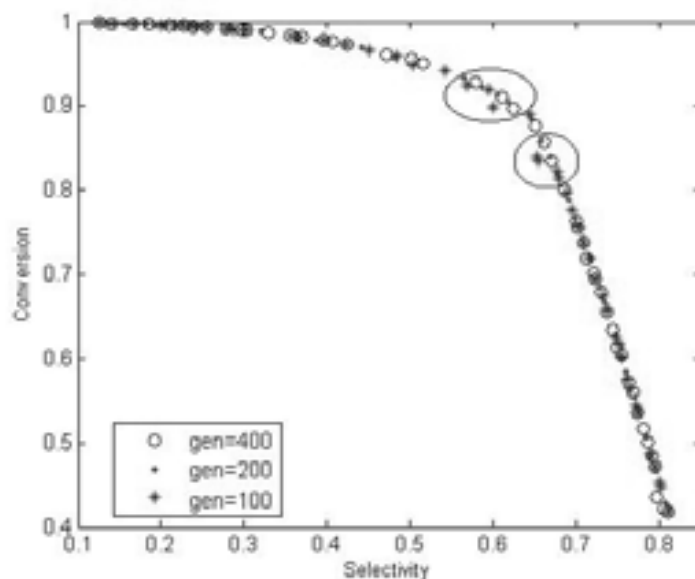


Figure 3. Effect of number of generations on Pareto front. $\eta_c = \eta_m = 0.01$, $N_{pop}=50$.

The effect of crossover and mutation probability distribution is depicted in Figure 4. The probability distribution index is a non-negative real number. A higher value of η_c allots a higher probability for creating near parent solutions and its small value permits

far-away solutions to be selected as offspring and speed of convergence. Whereas its lower value helps in the initial stages, when an exhaustive search is needed, convergence speed slightly decreases.

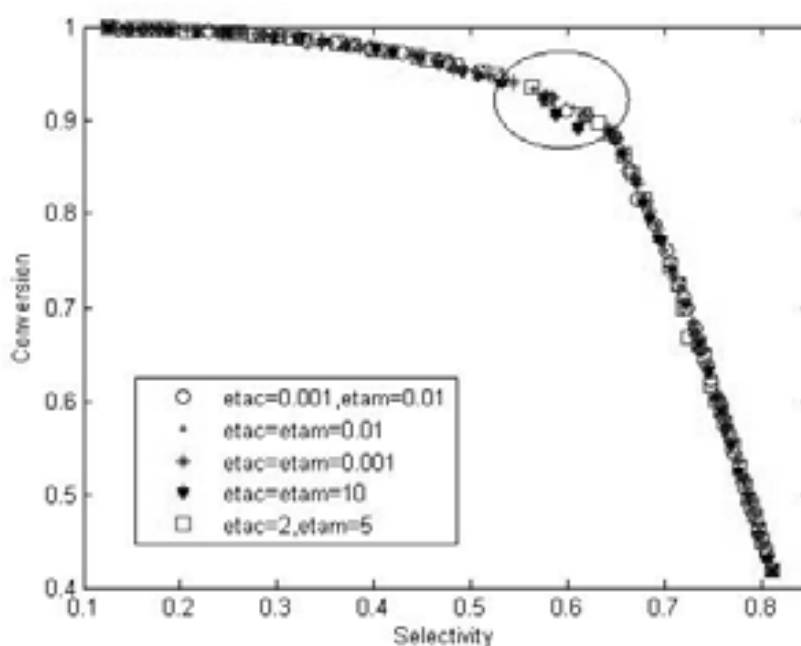


Figure 3. Effect of crossover and mutation probability distribution on Pareto front. $N_p=50$, $N_{gen}=200$.

Like η_c , the distribution index for polynomial mutation η_m is also a non-negative real number. The greater the value, the greater the change invariable. Figure 3 shows that decreasing η_c and η_m less than 0.01 results in only minor changes in the Pareto front. Therefore the value of 0.01 was selected for both distribution indexes. This shows that the Pareto obtained from all of these studies ultimately reach the same front, albeit with minor variations, mainly in Pareto ranges. This is an attribute of NSGA-II that has a low sensitivity to tunable parameters [18].

Among the Pareto fronts depicted in Figure 3, one representing set was found to be the widest and was plotted in Figure 2. It shows that, whereas the maximum ethane conversion had nearly reached 1, the maximum achievable selectivity was about 0.83.

It can also be observed in Figure 2 that as high conversion was achieved with moderate sacrifice in selectivity, achieving high selectivity required a much higher sacrifice in conversion. For a continuous process, the unreacted ethane can be separated and recycled back, but if ethane is converted to

any undesirable product, a loss is incurred. Thus, lower conversion is perhaps more acceptable than lower selectivity. On the other hand, if the process can be operated to recover side products such as propylene and butadiene, which are higher-value products, even high conversion might become a profitable option [19].

The best operating point can thus be determined after additional information, viz., the value of byproducts. The capital and operating costs, the controllability of the process variables, the results of hazard and safety analyses, etc., is made available and analyzed in a comprehensive way. The Pareto (Figure 2), however, brought out the intended outcome of multiobjective optimization, i.e., a wide range of competing options for operation.

6.3 - Decision variables corresponding Pareto front

Whereas the Pareto portrayed the competing nature of the objectives, the decision variables can be plotted against selectivity and conversion (Figures 4-5) to quantify their role in realizing the objective values.

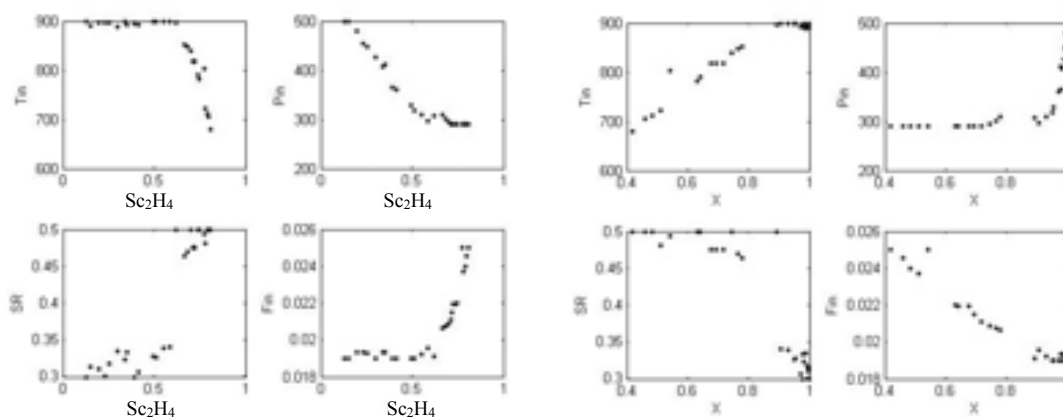


Figure 4. Decision variables corresponding to the Pareto in Figure 2.

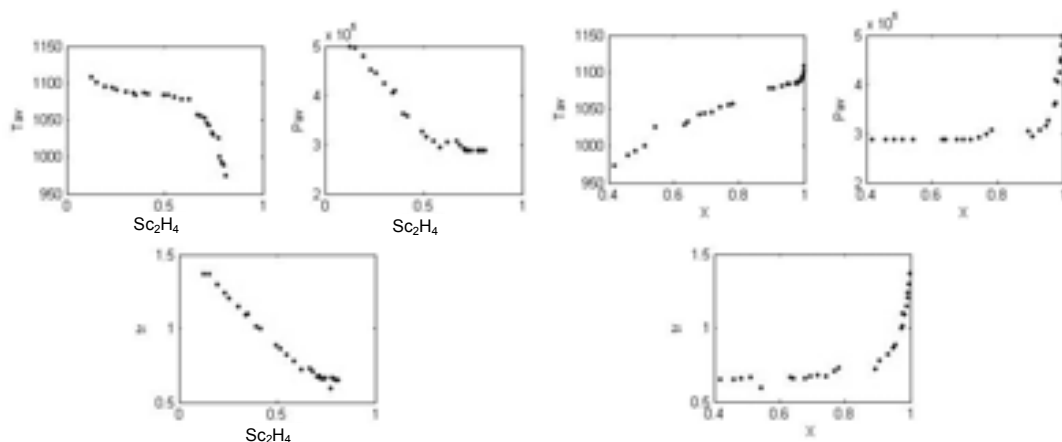


Figure 5. Some calculated variables (T_{av} , P_{av} , t_r) corresponding to the Pareto in Fig 2.

Moreover, they can be used to establish the fidelity of the optimization results as well. Figure 4 shows a decrease in the inlet temperature of the ethane-steam mixture with increasing selectivity, a behavior that was expected in light of the sensitivity analysis results.

The nature of the variation of the inlet feed flow rate complies with the findings in the sensitivity analysis section with relatively lower values for high conversion and higher values for high selectivity. The inlet pressure also has high values at lower selectivity and higher conversion. The high-pressure values toward very high conversions were probably chosen to increase the residence time and, as a result, the conversion.

The decision variable values in Figures 4 and 5, although having clear trends, are relatively scattered in nature when compared to the smooth variation of the Pareto front generated (Figure 2). This can be ascribed to the fact that more than one combination of multiple decision variables had similar effects on one or more of the objective values [19]. Minor scattering can be attributed to the compensatory effects on one another. For example, lower residence time (Figure 5) can be compensated by a high average temperature or a high average pressure, to

result in the same conversion.

7- Conclusion

Optimization of an ethane thermal cracking reactor using two objective functions such as ethane conversion and ethylene selectivity was successfully performed using a GA-based optimizer, NSGAI. The study produced a wide gamut of optimal operational options for the ethylene reactor, revealing a qualitative, as well as quantitative, relation of the reaction process with the operation variables. This demonstrated both the individual and combined roles played by reactor temperature, reactor pressure, and residence time in achieving the objectives. In general, a multiobjective optimization study is beneficial for understanding the performance tradeoff of conflicting objectives and decision variables and for producing a wide range of optimal solutions.

Nomenclature

C_p	heat capacity, J/mole K
d_t	tube diameter, m
F	molar flow rate, mole/hr
G	total mass flux of the process gas, kg/m ² s
$-\Delta H$	heat of reaction, J/mole

M_m	average molecular weight, kg/mole
N_{pop}	number of population
N_{gen}	number of generations
P_t	total pressure kPa
R	gas constant, J/mol k
R_b	radius of tube bend, m
Re	Reynolds number
r	reaction rate in Pyrolysis process, mole/m ³ s
s_{ij}	stoichiometry factor
T	temperature, K
z	axial reactor coordinate, m

Greek letters

η	unit conversion factor
η_c	crossover distribution parameter
η_m	mutation distribution parameter
ζ	parameter of tube bend
Λ	angle of bend in degree

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