

# Improving Cracking Severity in an Ethane Thermal Cracker Based on Dynamic Optimization Considering Process Limitations

**Razani, S.; Farsi, Mohammad\*<sup>+</sup>; Rahimpour, Mohammad Reza**

*Department of Chemical Engineering, School of Chemical and Petroleum Engineering, Shiraz University,  
Shiraz, I.R. IRAN*

**Bolhassani, A.**

*Jam Research and Development Center, Jam Petrochemical Complex,  
Bushehr, I.R. IRAN*

**ABSTRACT:** *The main goal of this research is to improve cracking severity in an industrial ethane thermal cracker in a domestic plant. In the first step, the considered cracker is modeled based on the mass and energy balance equations considering a molecular kinetic model. To develop an accurate model, a detailed thermal model is adopted to predict the tube skin temperature. To prove the accuracy of the developed model and considered assumptions, the simulation results are compared with the available plant data. In the next step, a sensitivity analysis is performed to investigate the effects of coil outlet temperature and steam to ethane ratio on the cracking severity factors including ethane conversion and production rate. Based on the results of sensitivity analysis although increasing steam to ethane ratio decreases ethane conversion, it improves ethylene yield. Then, a dynamic optimization problem is formulated to maximize ethylene production and minimize production decay during the process run time considering feed temperature, furnace temperature, and steam to ethane ratio as decision variables. The results show that applying the optimal condition to the system improves ethylene production by about 9.44%.*

**KEYWORDS:** *Ethane cracking; Molecular reaction network; Process modeling; Dynamic optimization.*

## INTRODUCTION

Ethylene is the simplest unsaturated hydrocarbon is the basic building block of many products such as polymers, chemicals, adhesives, detergents, and solvents [1, 2]. The main part of produced ethylene goes toward polyethylene, a widely used plastic containing polymer chains of ethylene units in various chain lengths.

Also, ethylene is used as a refrigerant, especially in LNG liquefaction plants. Thermal cracking and catalytic conversion are two main routes to convert different hydrocarbons such as gas oil, naphtha, LPG, and ethane to ethylene [3]. Although thermal cracking is a cyclic process with low product selectivity, and

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\* To whom correspondence should be addressed.

+ E-mail: [farsi@shirazu.ac.ir](mailto:farsi@shirazu.ac.ir)

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severe operating conditions, it is widely used in petrochemical plants due to the simple process.

The presented researches on the thermal cracking process could be classified into four categories including determination of reaction network and coke formation mechanisms, process modeling, and optimization. From the kinetic viewpoint, the free radical chain and molecular mechanisms are two main approaches to explain the chemistry of cracking reactions. Sundaram and Froment focused on the thermal cracking of ethane and propane and proposed two kinetic models based on the molecular and free radical mechanisms [4]. Although the free radical mechanism adequately predicted the experimental data, the main benefits of the molecular model were simplicity and ease of application. Belohlav et al. proposed a detailed molecular kinetic model to cover hydrogenation, aromatization, isomerization, and formal reactions in the ethane cracking process [5]. The results showed that an increasing number of reactions and components could improve the accuracy of molecular kinetic models. In general, most theoretical researches used molecular kinetic schemes due to simplicity and ease of application. Yan developed a steady-state model for an ethylene production plant and optimized the operating conditions of the process [6]. The results showed that separation and refrigeration units limit the production capacity in the considered plant. Based on the simulation results, applying the optimal conditions on the system increased gross profit by about 6% compared to the base case. *Caballero et al.* optimized the operating condition of an industrial ethane cracker to enhance the ethylene production rate [7]. The results showed that applying the optimal heat flux along the coil could increase ethane conversion and ethylene selectivity to 81.5% and 78.9%.

In general, coke builds up on the coil tube is a critical problem in the ethane crackers that has enormous effects on the process [8]. Typically, aromatics and unsaturated hydrocarbons such as ethylene, propylene, butene, and benzene are the most important coke precursors in the ethane cracking process. *Yancheshmesh et al.* simulated an industrial ethane cracker based on a molecular mechanism considering coke build-up on the coil tubes [9]. They investigated the effects of dilution type on the process performance. The results showed that mixing the feed stream with carbon dioxide as dilution increased ethylene production by decreasing coke builds up on the coil tube.

*Edwin and Balchen* focused on the production planning of a thermal cracker considering coke formation [10]. They calculated the dynamic trajectories of feed rate and steam concentration during the process run time to achieve maximum profit. Jiang and Du developed a multi-objective optimization problem dealing with feed scheduling in an ethane cracking unit to maximize the average benefits and minimize the coking rate considering cyclic schedules as decision variables [11]. The results showed that the average coking amount was lowered by about 4.20% in the optimized process compared to the conventional unit. *Barza et al.* modeled an ethane cracker in Arya Sasol Petrochemical Company based on the momentum, mass, and energy balance equations [12]. It was found that the developed model was capable to determine the process performance and coke deposition rate. *Zhou et al.* used an algebraic procedure to find the reaction network in the ethane cracking process [13]. They calculated the residence time in the cracker to achieve minimum by-product production. *Zaker et al.* modeled and optimized a naphtha thermal cracker at a dynamic state [14]. They formulated a single objective optimization problem to calculate the optimal trajectories of firebox temperature, feed temperature, and steam to naphtha ratio to achieve maximum ethylene capacity. They applied the genetic algorithm to solve the developed optimization problem. The results showed that applying optimal conditions to the system could increase the ethylene production rate from 15.31 to 15.49 ton/h.

In this study, an industrial ethane cracker is modeled based on the mass and energy balance equations considering a molecular mechanism. After sensitivity analysis, a multi-objective optimization problem is formulated considering operational constraints to enhance annual ethylene production and uniform production rate. Then, the objectives are combined with the weighted sum method and the dynamic trajectories of feed temperature, furnace temperature, and steam to methane ratio are determined during the process run time with the genetic algorithm as a powerful method in global optimization.

## PROCESS DESCRIPTION

In the considered thermal cracker, ethane is mixed with high-pressure steam and heated up to 530–630°C in the economizer. Steam as a dilution agent reduces the rate of reactions by decreasing the partial pressure of

hydrocarbons. On the other hand, it enhances ethylene selectivity and removes partially coke deposited on the coil tubes. The cracking reactions occur in the coil hanging at the centerline of the firebox. In the coil, the ethane molecules are cracked into ethylene and hydrogen. The outlet product feeds to the transfer line exchangers and is immediately cooled down to prevent over-cracking. Industrially, when the pressure drop in the coil or skin temperature reaches the critical levels, production is stopped and the coil is decoked. Fig. 1 shows the schematic diagram of an industrial cracker. Table 1 shows the design data of an ethane cracker and feed specification in Jam Petrochemical Complex.

## THEORETICAL SECTION

### Process modeling

In this section, the radiation section of an industrial cracker is modeled based on the mass and energy balance equations, and a dynamic framework is developed to investigate the process performance. To develop an accurate and simple mathematical model, some assumptions could be adopted as [15, 16]:

- Pseudo-steady state condition
- The uniform temperature in the firebox due to side burners
- The plug flow regime in the coil due to the high Reynolds number
- Ideal gas condition due to low pressure and high temperature
- Negligible axial heat and mass dispersions in the coil due to high Peclet number

Due to short residence time in the coil, the steady-state mass and energy balance equations could be written on an element of coil tube as:

$$\frac{dF_i}{dz} = \sum_{n=1}^N v_{i,n} r_{i,n} \left( \frac{\pi D_e^2}{4} \right) \quad (1)$$

$$F_i C_p \frac{dT}{dz} = U (T_f - T) (\pi D_e) + \sum_{n=1}^N r_n (-\Delta H)_n \left( \frac{\pi D_e^2}{4} \right) \quad (2)$$

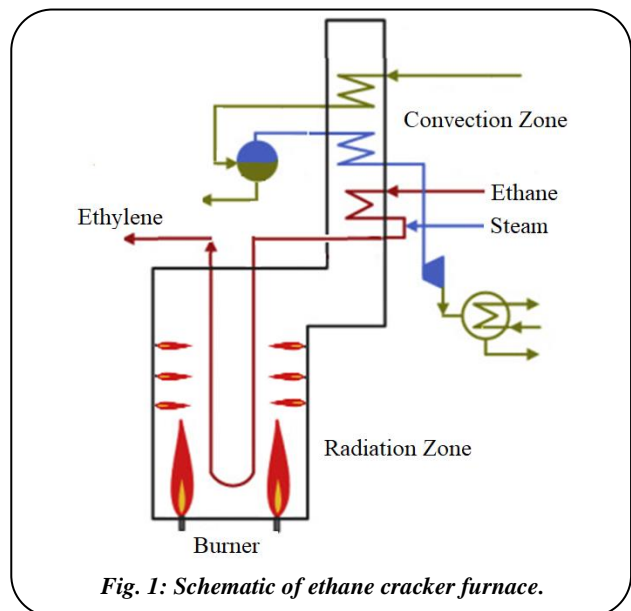
The pressure drop along the coil tube is calculated by:

$$-\frac{dP}{dz} = F_r \frac{G^2}{\rho_g} + G \frac{du_g}{dz} \quad (3)$$

Which the friction factor for straight tubes and bends are:

**Table 1: Specification of feed and cracker in Jam Petrochemical Complex**

Reactor design data	
Coil Length (m)	78
Number of passes	6
Inner Diameter (m)	0.1
Wall Thickness (m)	0.008
Feed specification and operating conditions	
Ethane flow rate (kg/h)	40047
Steam flow rate (kg/h)	12014
Feed temperature at SOR (K)	970.15
Feed temperature at EOR (K)	977.15
Feed pressure at SOR (bar)	3.09
Feed pressure at EOR (bar)	3.63
Furnace temperature at SOR (K)	1428.15
Furnace temperature at EOR (K)	1447.15



**Fig. 1: Schematic of ethane cracker furnace.**

$$F_r = \frac{0.092}{D_e} \frac{1}{Re^{0.2}} \quad (4)$$

$$F_r = \frac{0.092}{D_e} \frac{1}{Re^{0.2}} + \quad (5)$$

$$\frac{\xi \left( 0.07 + 0.035 \frac{\Lambda}{90} \right) \left( 0.051 + 0.19 \frac{D_i}{R_b} \right)}{\pi R_b}$$

The considered model to predict the effective diameter of coil tube is:

$$\rho_c \pi \frac{dD_e}{dt} = M w_c \sum_{j=1}^N v_j r_j \left( \frac{\pi D_e^2}{4} \right) \quad (6)$$

In the energy balance equation,  $U$  is the overall heat transfer coefficient and is explained as:

$$\frac{1}{U} = \sum_{i=1}^5 R_i \quad (7)$$

The considered heat transfer model includes convective heat resistance in the coil, conductive resistances in the deposited coke and tube material, and radiative and convective resistances in the firebox. The considered resistances are:

$$R_1 = \frac{1}{\pi D_e dz} \frac{1}{h_g} \quad (8)$$

$$R_2 = \frac{\ln \frac{D_i}{D_e}}{\pi dz} \frac{1}{k_{\text{coke}}} \quad (9)$$

$$R_3 = \frac{\ln \frac{D_o}{D_i}}{\pi dz} \frac{1}{k_{\text{coil}}} \quad (10)$$

$$R_4 = \frac{1}{\pi D_o dz} \frac{1}{h_g} \quad (11)$$

$$R_5 = \frac{1}{\pi D_o dz} \frac{1}{(T_{FB} + T_s)(T_{FB}^3 + T_s^2)} \quad (12)$$

### Kinetic Model

As mentioned, the kinetics of thermal cracking could be explained based on free radical and molecular mechanisms [17]. In this research, a molecular kinetic network consisting of 10 species and 12 elementary reactions is selected to predict the cracking severity and product distribution. Table 2 (a) and (b) provide the kinetic, rate equation and parameters of the considered kinetic model [9].

### Numerical solution

To solve the cracker model, the developed equation to calculate the effective diameter of the coil is discretized in the time domain, and steady-state mass and energy balance

equations are numerically solved in each time step by the fourth-order Runge Kutta method. The produced coke is deposited on the coil surface and the effective coil diameter is updated along the tube length. Typically, the produced heat in the firebox is transferred to the outer wall of the coil through the radiation and convection mechanisms. Then, heat is conducted along with the tube thickness and transferred to the feed by convection mechanism. The below procedure is considered to calculate the skin temperature in the furnace:

- Guess the skin temperature of element  $k$
- Calculate the rate of heat transfer between firebox and tube wall,  $Q_o^k$ .
- Solve the governing equations for element  $k$  and calculate the rate of heat transfer between the tube wall and gas phase,  $Q_i^k$ .
- If  $|Q_o^k - Q_i^k| > \epsilon$  correct the skin temperature
- Repeat the procedure for element  $k + 1$ .

### Process optimization

Generally, coke deposition on the coil tube and increasing thermal resistance in the system decrease ethylene production rate during the process run time in the industrial plants. In the industrial units, to overcome the production decay and uniform production rate, the temperature of the feed and firebox increases linearly during the process run time. In this regard, a multi-objective optimization problem is formulated considering annual ethylene production and uniform production rate as objective functions as:

$$J_1 = \int_0^{t_f} F_{C_2H_4} dt \quad (13)$$

$$J_2 = \int_0^{t_f} \left| F_{C_2H_4}^o - F_{C_2H_4}^t \right| dt \quad (14)$$

To simplicity, the considered objectives are combined with the weighted sum method and a single objective optimization problem is formulated [18]. The developed single objective problem could be explained as:

$$J_1 = \omega_1 \int_0^{t_f} F_{C_2H_4} dt + \omega_2 \int_0^{t_f} \left| F_{C_2H_4}^o - F_{C_2H_4}^t \right| dt \quad (15)$$

Where

$$\omega_1 + \omega_2 = 1 \quad (16)$$

Table 2(a), The kinetic and rate equation of the considered model.

Reactions	Rate equations
$C_2H_6 \leftrightarrow C_2H_4 + H_2$	$r_1 = k_1 \left[ \frac{F_{C_2H_6}}{F_t} \left( \frac{P_t}{RT} \right) \right] - k_{-1} \left[ \frac{F_{C_2H_4} F_{H_2}}{F_t^2} \left( \frac{P_t}{RT} \right)^2 \right]$
$2C_2H_6 \rightarrow C_3H_8 + CH_4$	$r_2 = k_2 \left[ \frac{F_{C_2H_6}}{F_t} \left( \frac{P_t}{RT} \right) \right]$
$C_3H_8 \leftrightarrow C_3H_6 + H_2$	$r_3 = k_3 \left[ \frac{F_{C_3H_8}}{F_t} \left( \frac{P_t}{RT} \right) \right]$
$C_3H_8 \rightarrow C_2H_4 + CH_4$	$r_4 = k_4 \left[ \frac{F_{C_3H_8}}{F_t} \left( \frac{P_t}{RT} \right) \right]$
$C_3H_6 \rightarrow C_2H_2 + CH_4$	$r_5 = k_5 \left[ \frac{F_{C_3H_6}}{F_t} \left( \frac{P_t}{RT} \right) \right] - k_{-5} \left[ \frac{F_{C_2H_2} F_{CH_4}}{F_t^2} \left( \frac{P_t}{RT} \right)^2 \right]$
$C_2H_2 + C_2H_4 \rightarrow C_4H_6$	$r_6 = k_6 \left[ \frac{F_{C_2H_2} F_{C_2H_4}}{F_t^2} \left( \frac{P_t}{RT} \right)^2 \right]$
$2C_2H_6 \rightarrow C_2H_4 + 2CH_4$	$r_7 = k_7 \left[ \frac{F_{C_2H_6}}{F_t} \left( \frac{P_t}{RT} \right) \right]$
$C_2H_6 + C_2H_4 \rightarrow C_3H_6 + CH_4$	$r_8 = k_8 \left[ \frac{F_{C_2H_6} F_{C_2H_4}}{F_t^2} \left( \frac{P_t}{RT} \right)^2 \right]$
$C_2H_4 \rightarrow \text{Coke}$	$r_9 = k_9 \left[ \left( \frac{F_{C_2H_4} P_t}{F_t RT} \right)^{1.34} \right]$
$C_3H_6 \rightarrow \text{Coke}$	$r_{10} = k_{10} \left[ \left( \frac{F_{C_3H_6} P_t}{F_t RT} \right)^{1.34} \right]$
$C_4H_6 \rightarrow \text{Coke}$	$r_{11} = k_{11} \left[ \left( \frac{F_{H_2O} P_t}{F_t} \right) \right]$
$\text{Coke} + H_2O \rightarrow CO + H_2$	$r_{12} = k_{12} \left[ \left( \frac{F_{H_2O} P_t}{F_t} \right) \right]$

Table 2(b): Arrhenius parameters for reaction.

Rate coefficient	A $\left( \frac{m^3}{mol s} \right)$	E $\left( \frac{j}{mol} \right)$
$k_1$	$4.65 \times 10^{13}$	$2.73 \times 10^5$
$k_2$	$3.85 \times 10^{11}$	$2.73 \times 10^5$
$k_3$	$5.89 \times 10^{10}$	$2.15 \times 10^5$
$k_4$	$4.69 \times 10^{10}$	$2.12 \times 10^5$
$k_5$	$6.81 \times 10^8$	$1.54 \times 10^5$
$k_6$	$1.03 \times 10^9$	$1.73 \times 10^5$
$k_7$	$6.37 \times 10^{23}$	$5.3 \times 10^5$
$k_8$	$7.08 \times 10^{10}$	$2.53 \times 10^5$
$k_9$	$5.00 \times 10^{14}$	$2.24 \times 10^5$
$k_{10}$	$2.77 \times 10^9$	$1.16 \times 10^5$
$k_{11}$	$5.61 \times 10^{18}$	$2.74 \times 10^5$
$k_{12}$	$5.09 \times 10^4$	$2.38 \times 10^5$
$k_{,1}$	$8.49 \times 10^8$	$1.36 \times 10^5$
$k_{,5}$	$3.81 \times 10^8$	$1.47 \times 10^5$

**Table 3: Comparison between simulation results and taken data from a domestic Plant.**

	Start of Run			End of Run		
	Plant Data	Simulation	Absolute Relative Error (%)	Plant Data	Simulation	Absolute Relative Error (%)
COT (K)	1118	1102.4	1.40	1118	1106.6	1.02
Pressure (Bar)	2.12	2.16	1.89	2.13	2.07	2.82
Ethane (mole/s)	123.34	124.49	0.94	131.51	132.09	0.44
Ethylene (mole/s)	206.97	206.95	0.10	201.23	199.73	0.74

$$\text{Absolute Relative Error} = \frac{X_{\text{Plant}} - X_{\text{Model}}}{X_{\text{Plant}}} \times 100$$

The value of considered weights is arbitrary and selected based on the operator's decision. In this research, the values of  $w_1$  and  $w_2$  are 0.5 and 0.5, respectively. To find the optimal trajectories of decision variables, the process run time is divided into four time periods and a time-dependent linear polynomial is considered for each decision variable. Then the optimal values of coefficients are determined in each period based on the formulated optimization problem by genetic algorithm considering the continuity of feed and furnace temperatures in the process run time as a constraint. To prevent cracking and coke build-up in the economizer, the maximum feed temperature is set to be 1000K. Besides, 1380K is selected as the upper bound of skin, temperature to prevent coil melting, and safety limitations. Although increasing steam concentration in the feed stream improves the ethylene yield, it increases operating costs. Thus, the molar steam to ethane ratio is fixed in the range 0.5-0.8. Based on the plant strategy and facilities, the maximum pressure drop in the coil is set to be 2 bar. Also, according to the operating condition of a conventional cracker, the process run length is set to be 60 days. The considered bounds and constraints are [19]:

$$T_{\text{Feed}} < 1000 \text{ K} \quad (17)$$

$$= T_{\text{Furnace}} < 1500 \text{ K} \quad (18)$$

$$T_{\text{Skin}} < 1380 \text{ K} \quad (19)$$

$$0.5 < \text{Molar Steam to Ethane Ratio} < 0.8 \quad (20)$$

$$\text{Coke Thickness} < 1 \text{ cm} \quad (21)$$

$$\Delta P < 2 \text{ bar} \quad (22)$$

In this research, the formulated optimization problem is handled by the Genetic algorithm as a powerful method in global optimization.

## RESULTS AND DISCUSSION

### Model Validation

In this section, to prove the accuracy of the developed model and considered assumptions, the simulation results are compared with the available plant data. Table 3 presents the comparison between simulation results and taken data from a domestic ethylene plant [7]. The small absolute relative difference of simulation results and plant data proves the accuracy of the model.

### Sensitivity Analysis

In this section, a sensitivity analysis is performed to investigate the effects of operating temperature and steam concentration on the cracking severity. From an industrial viewpoint, the coil outlet temperature is a practical indicator to estimate and control the cracking severity [20]. In this regard, the effects of coil outlet temperature and steam to ethane ratio on the ethane conversion and ethylene production rate are investigated with the developed model. Fig. 2(a) and (b) show the effects of coil outlet temperature on the ethylene production rate and ethane conversion, respectively. Typically, the desired coil outlet temperature could be developed by changing both feed and furnace temperatures. Based on the simulation results, increasing coil outlet temperature improves cracking severity and results in higher ethylene production. It appears changing feed temperature to raise the coil outlet temperature from 1102.5 K to 1120 K improves ethane conversion from 66.35% to 79.25%, while changing firebox temperature enhances conversion from 66.35% to 75.65%. Although the manipulation of feed temperature is more effective to enhance ethylene production and ethane conversion compared to the furnace temperature, increasing feed temperature results in over-cracking and coke formation in the preheater.

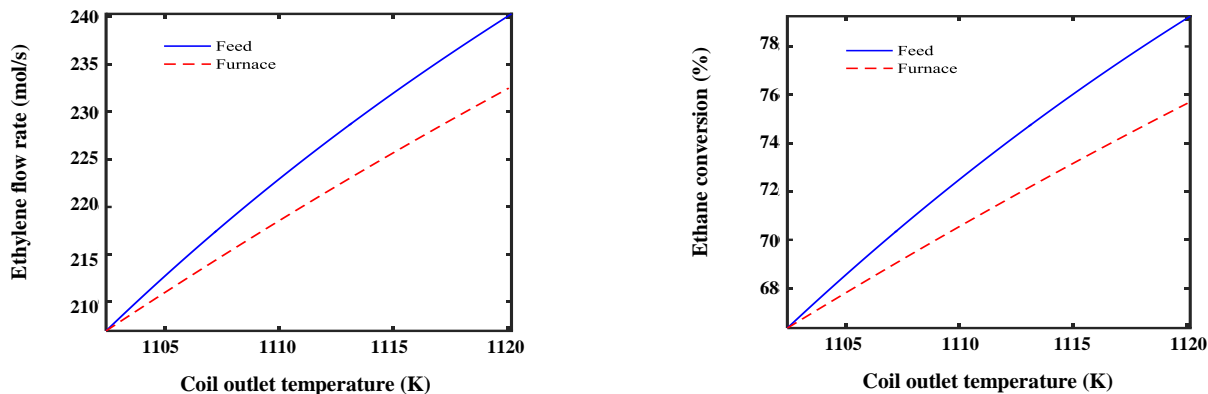


Fig. 2: a) Effect of coil outlet temperature on ethylene production. b) Effect of coil outlet temperature on ethane conversion.

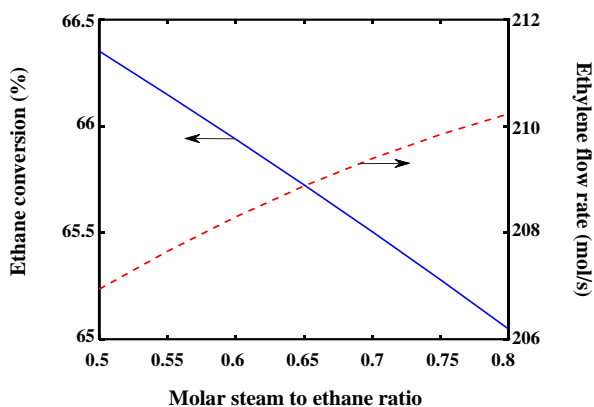


Fig. 3: Effect of steam to ethane ratio on ethylene production and ethane conversion.

It concludes from the presented results that the product distribution and cracking severity are path-dependent.

Fig. 3 shows the effects of steam to ethane ratio on ethylene production and ethane conversion, respectively. In the thermal cracking units, the suitable mass ratio of steam to hydrocarbon varies in the range of 0.2–1.0 [21]. Low steam to hydrocarbon ratio is favorable in the case of light feedstocks such as ethane. Steam decreases the rate of cracking reactions by reducing the hydrocarbon partial pressure and improves the ethylene selectivity by decreasing residence time in the coil. Based on the simulation results, although increasing the steam to ethane ratio from 0.5 and 0.8 decreases ethane conversion from 66.35% to 65.05%, it increases ethylene yield from 84.3% to 87.36%. It concludes that increasing steam concentration in the feed stream improves ethylene production and yield in the ethane cracking process.

### Process Optimization

In the thermal cracking process, ethane is converted to a wide range of products such as hydrogen, methane, ethylene, and propylene. Typically, coke deposition on the coil surface and decreasing the effective diameter of the coil, tube reduces ethylene production capacity, continuous run length, and outlet pressure. In this section, the calculated optimal trajectories of feed temperature, furnace temperature, and steam to ethane ratio are presented to achieve maximum cracking performance. The molar steam to ethane ratio at the conventional and optimal conditions are 0.5 and 0.8, respectively. Fig. 4 (a) and (b) show the calculated trajectories of feed and furnace temperatures at the conventional and optimal conditions. In this research, to find the optimal trajectory of decision variables, the process run time is divided into four time periods and a time-dependent linear polynomial is considered for each decision variable in each period. Then the optimal values of coefficients are determined in each period based on the formulated optimization problem by genetic algorithm. Thus, the appeared breakpoints are due to the change in the slope of the polynomials. Generally, increasing steam concentration in the feed, steam decreases the rate of coke formation in the coil tube and permits applying the higher feed and furnace temperatures on the system to increase ethylene production capacity and uniform production rate.

Fig. 5 (a) shows ethylene production capacity during the process run time. As well as higher ethylene production, the uniform production rate is another benefit of the optimized process. The ethylene production rate decreases from 207 to 199.7 mole/s in the conventional process, when the production decay in the optimized

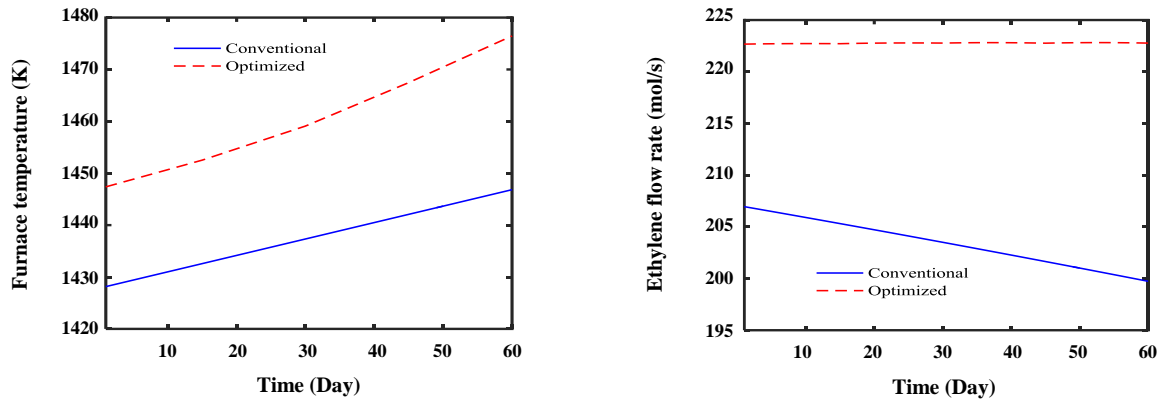


Fig. 4: a) Calculated dynamic trajectory of furnace temperature. b) Calculated dynamic trajectory of feed temperature.

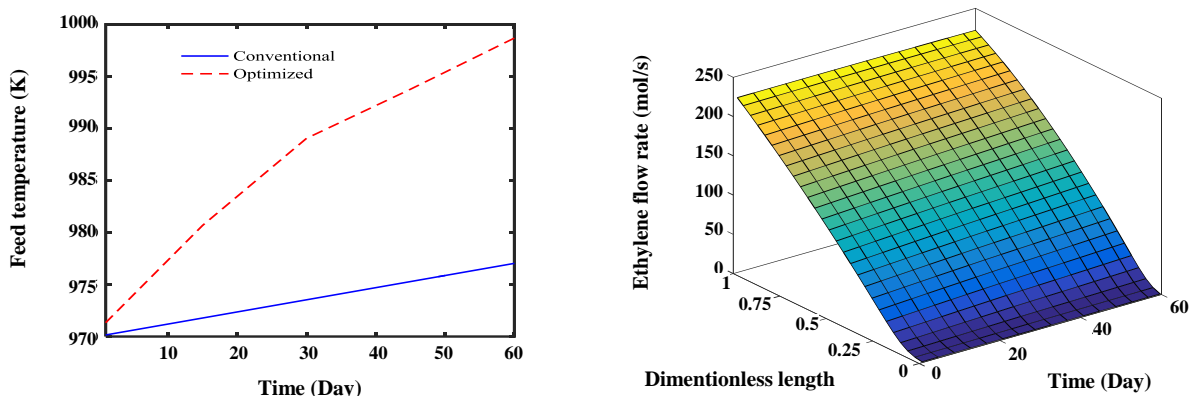


Fig. 5: a) Ethylene production capacity at the optimized and conventional conditions. b) Ethylene flow rate along with the coil during the process run time at optimized condition.

the process is negligible. It appears that the mean ethylene production rate at the optimized and conventional conditions are 222.8 mole/s and 203.42 mole/s, respectively. Based on the simulation results, the annual ethylene production capacity increases by about 17112.7 tons by applying the obtained optimal conditions on the system. In other words, ethylene production is improved by 9.44% applying optimal trajectories on the cracker.

Figs. 5(b) shows the molar flow rate of ethylene along the cracker length during the process run time at the optimized condition. Typically, the inlet feed stream to the coil is preheated in the convection section of the cracker. Increasing feed temperature in the preheater promotes the rate of cracking reactions and results in the coke formation in the preheater. Thus, the lowest rate of ethylene production appears at the entrance of the coil tube where the lowest temperature is observed. Since the coil

is surrounded by a firebox, the generated heat in the firebox is transferred to the coil, and the ethylene production rate increases along with the coil linearly.

Fig. 6 (a) and (b) show ethane conversion and ethylene yield during the process run time at the conventional and optimized conditions. Both reaction yield and conversion are the main parameters to analyze the performance of crackers and represent the cracking severity. Ethylene yield is defined as the produced ethylene per mole of consumed ethane through cracking reactions. It appears that applying optimal conditions on the system improves ethane conversion in the cracker. Based on the simulation results, the ethane conversion at the optimized and conventional conditions is 70.01% and 65.37%, respectively. Besides, applying the optimal trajectories on the system increases ethylene yield from 84.11% to 85.95% compared to the conventional condition.



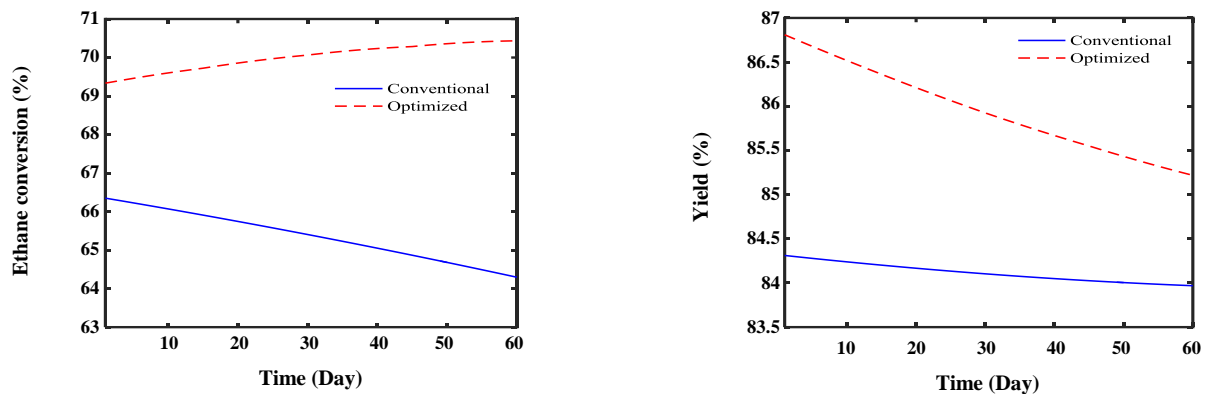


Fig. 6: a) Ethane conversion at the optimized and conventional conditions.  
b) Ethylene yield at the optimized and conventional conditions.

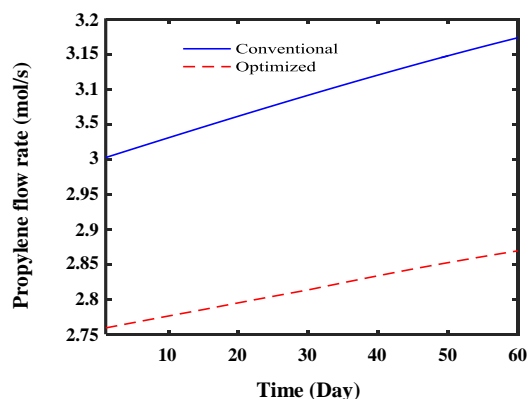


Fig. 7: Propylene production capacity at the optimized and conventional conditions.

Fig. 7 shows the molar flow rate of propylene as a valuable by-product during the process run time. Based on the considered reaction network, ethane is cracked into propane and methane. The propylene could be produced through propane dehydrogenation and methylation of ethane and propane. It appears that propylene production at the optimized and conventional conditions are 2.82 mole/s and 3.09 mole/s, respectively. Based on the simulation results, annual propylene production decreases by about 347.8 tons by applying the optimal condition on the system.

Fig. 8(a) and (b) show the operating temperature and coil outlet temperature profiles during the process run time, respectively. Although cracking reactions are endothermic, the heat transfer from the firebox to the coil is dominant and the temperature increases along the tube length. Also, increasing the temperatures of feed and

firebox to overcome the effects of coke build-up increases coil outlet temperature in the system. It appears that the maximum value of coil outlet temperature is about 1127K at the optimized condition, which is in the range of industrial crackers [22].

Fig. 9(a) and (b) show the skin temperature during the process run time. Generally, skin temperature is one of the main constraints in the cracking units that limits production capacity. Typically, increasing temperatures of feed and firebox and coke builds up in the coil increase skin temperature during the process run time. Based on the simulation results, the skin temperature is in the range of 1290 to 1345 K at the conventional condition, and applying the optimal condition on the system increases skin temperature up to 1375K. It is mentioned that the considered upper bound of skin temperature in the ethane cracker is 1380 K.

Figs. 10 and 11 show the effective coil diameter and pressure profiles at the optimal condition. Based on the considered kinetic model, the olefinic compounds are thermally converted to coke. The produced coke is deposited in the coil tube and decreases the effective diameter of the coil. The most coke thickness is appeared in the last part of the coil due to the high concentration of olefinic components and high temperature. The produced coke decreases the heat transfer coefficient in the system and increases the pressure drop in the coil. When the pressure drop in the coil and inlet pressure reaches the critical values, the process is stopped and the coil is decoked by a mixture of air and steam. It appears that increasing feed pressure could maintain the outlet pressure

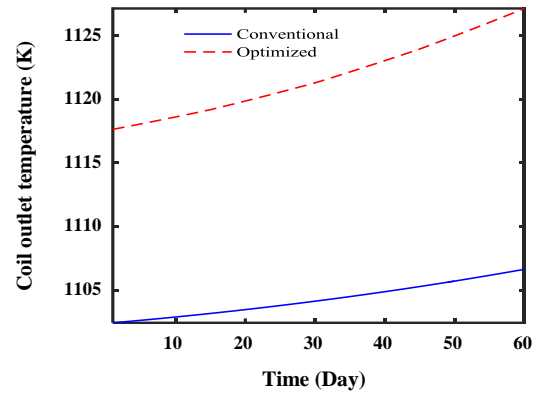
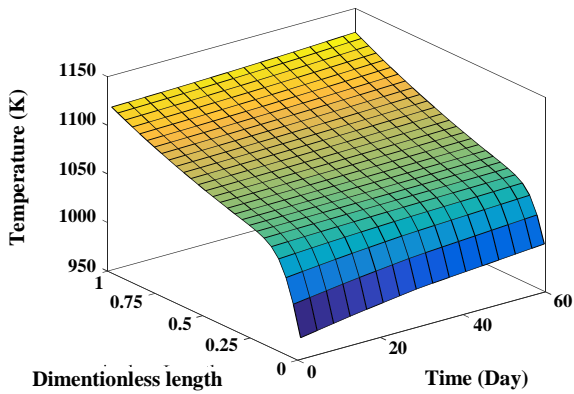


Fig. 8: a) Temperature profile along the coil at optimized condition. b) Outlet coil temperature at the optimized and conventional conditions.

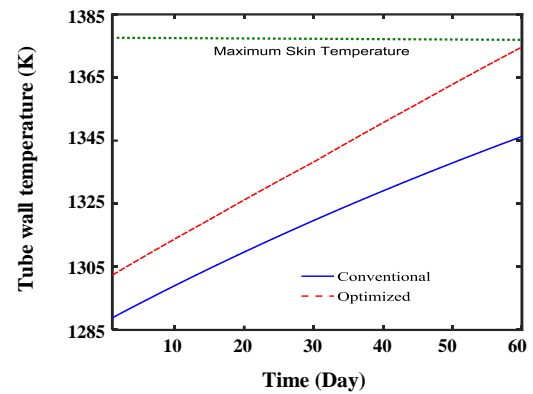
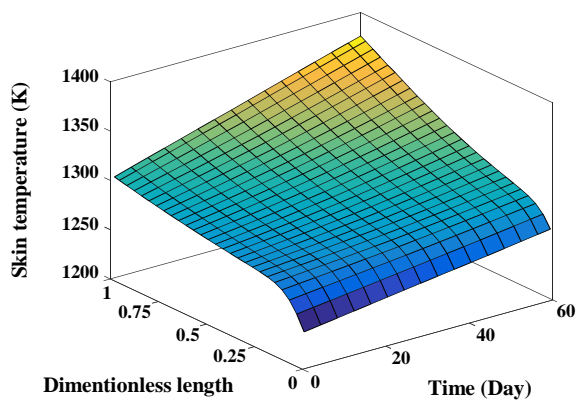


Fig. 9: a) Skin temperature along the coil during the process run time at optimized condition. b) Maximum skin temperature at the optimized and conventional conditions.

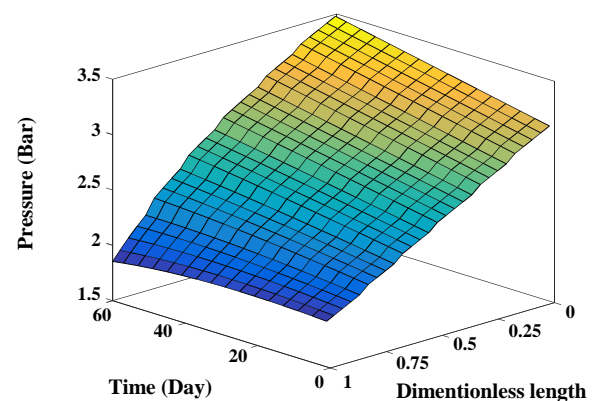
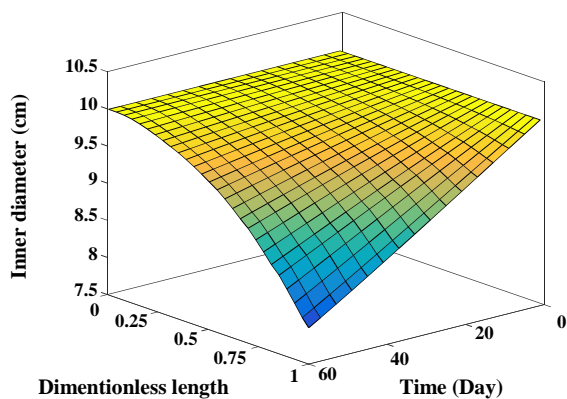


Fig. 10: Effective coil diameter at optimized condition.

Fig. 11: Pressure profile along the coil tube at optimized condition.

as the desired condition. Based on the plant datasheet a six-pass coil is applied in the considered ethane cracker. The appeared ribbing in the pressure profile is due to bends ( $180^\circ$ ) where the fluid direction changes in the coil.

## CONCLUSIONS

In this research, an industrial ethane cracker was modeled and simulated based on the mass and energy balance equations considering a detailed thermal model.

The accuracy of the developed model was proved against plant data. The results of sensitivity analysis showed that increasing the steam to ethane ratio in the feed stream enhanced ethylene yield. To improve the performance of ethane crackers, a multi-objective optimization problem was formulated considering annual ethylene production and uniform production rate as objective functions. The objectives were combined with the weighted sum method and the optimal trajectories of feed temperature, furnace temperature, and steam to ethane ratio were determined during the process run time. Based on the simulation results, applying the optimal condition on the system increased the annual ethylene production by about 17112.7 tons. Although ethane conversion and ethylene yield were improved by about 7.01% and 2.19% in the optimized process, it decreased annual propylene production by about 347.8 tons compared to the conventional cracker.

#### Nomenclature

C	Concentration, mol/m <sup>3</sup>
C <sub>p</sub>	Heat capacity, J/mol.K
D <sub>t</sub>	Effective coil diameter, m
F <sub>i</sub>	The molar flow rate of component i, mole/s
F <sub>t</sub>	Total flow rate, mole/s
F <sub>r</sub>	Friction factor
G	Total mass flow rate, kg/m.s
h	Heat transfer coefficient, W/m <sup>2</sup> .K
J	Objective function
k	Thermal conductivity, W/m.K
k <sub>i</sub>	Rate coefficient of reaction i, s <sup>-1</sup> or m <sup>3</sup> /mol.s
M <sub>w</sub>	Molecular weight, kg/mol
N	Number of reactions
P	Pressure, Pa
Q	Heat flux, W/m <sup>2</sup>
R <sub>c</sub>	Rate of coking, mol/m <sup>2</sup> .s
r <sub>i</sub>	Rate of reaction i, mol/m <sup>2</sup> /s
R	Universal gas constant, J/mol.K
R <sub>i</sub>	Thermal resistance, k/W
R <sub>b</sub>	The radius of tube bend, m
Re	Reynolds number
v <sub>i,n</sub>	Stoichiometric coefficient of component n in i <sup>th</sup> reaction
T	Temperature, K
t	Time, s
U	Overall heat transfer coefficient, J/mol.K
u <sub>g</sub>	Gas velocity, m/s

w	Weight of objectives
z	axial reactor coordinate, m

#### Greek letters

ΔH	Heat of reaction, kJ/mol
ΔP	Pressure drop, Pa
ξ	Tube bend parameter
σ	Boltzmann constant
Λ	Bend angel
α	Coking factor
ρ	Specific gravity, kg/m <sup>3</sup>

#### Subscripts

c	Coke
F	Feed
FB	Firebox
g	Gas
s	Skin

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