ABSTRACT: With the global production of 150 million tons in 2016, ethylene is one of the most significant building blocks in today’s chemical industry. Most ethylene is now produced in cracking furnaces by thermal cracking of fossil feedstocks with steam. This process consumes around 8% of the main energy used in the petrochemical industry, making it the single most energy-intensive process in the chemical industry. This paper studies a tubular thermal cracking reactor fed by propane and the molecular mechanism of the reaction within the reactor. After developing the reaction model, the existing issues, such as the reaction, flow, momentum, and energy, were resolved by applying heat to the outer tube wall. After solving the entropy generation equations, the entropy generation ratio of the sources was evaluated. The temperature of the tube/reactor was tuned following the reference results, and processes were replicated for different states. The verification of the modeling and simulation results was compared with the industrial case. The Genetic Programming (GP) machine learning approach was employed to generate objective functions based on key decision variables to reduce the computational time of the optimization algorithm. For the first time, this study has proposed a systematic approach for optimizing a thermal cracking reactor based on a combination of Genetic Programming (GP), Water Cycle Algorithm (WCA), and Genetic Algorithm (GA). In this regard, multiobjective optimization was performed based on the maximization of the products and entropy generation with the generation of GP objective functions. The key decision variables in this study included inlet gas temperature, inlet gas pressure, air mass flow rate, and wall temperature. The results showed that the weighted percentage of products after optimization increased to 61.13% and the entropy production rate of the system decreased to 899.80 J/s, displaying an improvement of 0.85 and 16.51% compared with the base case, respectively, with the multiobjective GA algorithm. In addition, by applying the multiobjective WCA, the weighted percentage of products increased to 61.81%. The entropy production rate of the system decreased to 882.72 J/s. So, an improvement of 1.97% in weights of products and an improvement of 18.77% in entropy generation have been achieved compared with the base case.

1. INTRODUCTION

The thermal cracking of hydrocarbons is the most common form of olefin production. The thermal cracking of propane is conducted using a radical mechanism that is highly studied and researched by Zhou et al., who conducted an entropy generation minimization in a solid reactor based on construction theory; their model consisted of 10 reactions. The molecular model of reactions performs quickly and is broadly applied in ref for the simulation of propane thermal cracking. An industrial cracker was simulated in ref using the presented scheme. They developed a molecular model for nine reactions with nine components. Masoumi et al. studied the thermal cracking furnace and monitored its dynamic behavior. To this end, they built a pilot plant controlled by a computer system. The steady-state model had one dimension, 543 reactions, and 90 elements.

They intended to enhance the steady-state to gain maximum advantage. Gao et al. modeled the tubular reactor in a naphtha cracking furnace to optimize it using the HYSYS software package. Their method also enhanced the operation profitability considerably. Process assessment was conducted under steady-state circumstances. However, the real-world coke formation is time-dependent, affecting the efficiency; they did not consider coke thickness in the heat transfer coefficient.
Ghasemi et al.\textsuperscript{7} used a 3D model and computational fluid dynamics to study the ethylene furnace. The temperatures of the tube skin and heat flux profiles were measured by solving the mass, momentum, and energy equations corresponding to furnaces in ANSYS Fluent. The results indicated that by increasing the fuel rate, outlet propylene yield decreased, while process gas temperature, pressure drop, propane conversion, and ethylene yield were increased along the reactor tube. In addition, increasing reactor feed flow rate increased the desired product yields, despite the reduction in the coil outlet temperature of the reactor.

Ghazheae and Karimzadeh\textsuperscript{5} attempted to use a dynamic model to explain why cracks show an unsteady-state behavior during their start-up in furnaces. Their mathematical model, the convection model, comprised four sub-models: cylindrical coil, combustion chamber, and shell and tube. They captured a two-dimensional zone to predict the factors at a start-up run using these four sub-models. Zheng et al.\textsuperscript{6} calculated the heat flow and temperature distribution using CFD 3D modeling in the thermal cracking reactor and furnace and compared the results using spectrometry. Barazandeh et al.\textsuperscript{7} investigated a liquid furnace cracking reactor and furnace and compared the results using CFD 3D modeling in the thermal reactor using optimal control theory. They considered temperature a control variable and used governing equations of the plug flow reaction and SO\textsubscript{2} oxidation to show a way to minimize the entropy generation rate in plug flow reactors by optimal control theory. It is demonstrated that decreasing the entropy generation rate up to 25\% can be obtained by changing the reactor length and controlling the utility. A hypothesis was proposed that a reactor with high energy efficiency had relatively long sections with constant entropy generation rate and driving forces.

Kingston and Razzite\textsuperscript{17} investigated the unique kinds of continuously stirred tank reactors (CSTRs) and plug flow reactors (PFRs). They also verified the temperature and pressure and gave a graphical picture of entropy generation in chemical reactions to constant volume, allowing access to different options efficiently. Also, they indicated that by dividing a reactor into two smaller ones, with different operating temperatures, the entropy generation decreased, going near as 48\% less in the case of a CSTR and PFR in series, and achieving 58\% with two CSTR.

Chen et al.\textsuperscript{18} produced light olefins using CO\textsubscript{2} hydrogenation to minimize entropy production. Røsjorde et al.\textsuperscript{19} attempted to minimize entropy production in propane dehydrogenation using different tower condenser reactor and exchanger components. The structural theory to model and minimize entropy generation has been used. Abdous et al.\textsuperscript{20} analyzed the same problem in helically coiled tubes under flow boiling conditions under a constant heat flux. Kurnia et al.\textsuperscript{21} applied this analysis to various cross-sections.

Vandewalle et al.\textsuperscript{22} used computational fluid dynamic (CFD) fouling in steam cracking reactors and developed a 3D algorithm to simulate coke formation in steam cracking reactors. They examined coke layer growth to analyze a reactor’s run length and determined that the ribbed reactor design had the most extended run length.

Mu and Gu\textsuperscript{23} studied the optimal modeling of thermal cracking furnaces based on the enriched Kumar model by considering free-radical reactions. An improved search engine algorithm (IPR) was developed to compute the importance of substances in the Kumar model for efficient model selection. The proposed model indicated that the new model achieved a mean relative error (MRE) of less than 0.1\% compared to 5\% in the Kumar model. The proposed model could be applied to modeling extensive feedstocks with high accuracy.

Zhou et al.\textsuperscript{24} optimized the ethane thermal cracking furnace via the coupling of the reaction network. The residence time related to the minimum by-product was determined to be 0.4 s, and its by-product was 4.3\% less than that at the initial residence time (0.3 s).

Gold yttrium oxide nanorods for oxidative catalytic cracking of \(\alpha\)-propane to light olefins have been studied by Narasimharao and Alshehri.\textsuperscript{25} Gold nanoparticles loading has affected the activity of oxidative catalytic cracking. In addition, simple Au-O-Y species and Lewis acid sites are provided for the activity.

Ebrahimian et al.\textsuperscript{26} proposed an innovative reactor concept for thermal coupling of naphtha reforming with propane amnoniation. The production of aromatics, hydrogen, and acrylonitrile have been considered. The evaluation of the thermally coupled reactors with the conventional reactors has been performed—eliminating traditional furnaces in naphtha reforming.
A comprehensive investigation on hydrogen production through propane steam reforming inside a reactor has been performed by Barnoon et al.\textsuperscript{37} The results demonstrate that the hydrogen generation yield can change from 77.5 to 92.2%. The reaction rate can be varied by the velocity and temperatures of the hot gases. Also, for $T = 900$ K, full propane used is obtained at the reformer outlet.

Simulation and dynamic optimization to find optimum operational parameters of the industrial tubular reactor for propane cracking have been investigated by Berreni and Wang.\textsuperscript{28} This work was performed in gPROMS. The steady-state and dynamic optimizations were respectively performed. The results show that dynamic optimization can improve the net profit by 10.6% rather than the base case. In addition, the computation demand by dynamic optimization was much wider and higher than the steady-state optimization.

A coupled CFD simulation method for investigating the pyrolysis process in industrial naphtha thermal cracking furnaces has been performed by Rezaeimanesh et al.\textsuperscript{29} A typical $k$–$\varepsilon$ turbulence model is combined with the molecular kinetic response for cracking, a thorough combustion model, and radiative properties in this full CFD model. The simulation results corresponded well with industrial data acquired from a mega olefin plant of a petrochemical complex in terms of temperature, product yield, and especially propylene-to-ethylene ratio (P/E). The difference between P/E resulting from industrial data was less than 2%.

From the standpoint of intelligent manufacturing, knowledge expression, numerical modeling, and optimization application of ethylene thermal cracking have been investigated by Zhang et al.\textsuperscript{32} This study presented a summary of advances and ethylene thermal cracking have been investigated by Zhang et al.\textsuperscript{30} The results demonstrated that the hydrogen generation yield can change from 77.5 to 92.2%. The reaction rate can be varied by the velocity and temperatures of the hot gases. Also, for $T = 900$ K, full propane used is obtained at the reformer outlet.

Figure 1. Hydrocarbon thermal cracking process.\textsuperscript{34}

For an ethylene-cracking furnace with many faults and exceptional operation conditions, a two-level completely energy-efficient quantitative diagnosis method was developed by Meng et al.\textsuperscript{33} The goal of energy efficiency diagnosis was to determine the severity and root causes of various types of inefficiency. More accurate findings are obtained when a mechanism and a data-driven multiple benchmark criteria are coupled.

Saffari et al.\textsuperscript{34} assessed the entropy generation in a thermal cracking reactor. The results indicated for two states that the three factors were in the order of chemical reactions, heat transfer, and pressure loss in terms of their contribution to entropy generation. The variation of feed temperature did not affect the entropy generated by the chemical reactions. However, the entropy generation in the reactor with optimum wall temperature was the lowest. Also, entropy was higher at the inlet of the reactor when the wall had an optimal temperature.

Previous studies rely on basic principles of flow, chemical reactions, and fundamental energy equations, which do not involve minimization of entropy generation and its adequation for the process. A review of previous research shows no investigation of optimizing thermal cracking reactors by addressing maximum productivity and minimum entropy generation. In addition, no systematic approach has been adopted for the multiobjective optimization of thermal cracking reactors. The innovation of this study is that it has, for the first time, addressed the maximization of productivity, and minimization of entropy generation have been considered simultaneously. In this regard, the second law of thermodynamics and the entropy production rate were employed. Considering entropy generation sources, the basic factors, and mitigating its generation, enhance the process that may lead to a better economization. Also, a systematic approach was adopted based on the genetic programming (GP) technique for the multiobjective optimization of thermal cracking reactors based on key parameters based on minimizing entropy generation and maximizing products. The GP technique reduced the run time and obtained high convergence to two objectives optimization.

### 2. THERMAL CRACKING PROCESS

Lighter product yield when the hydrocarbon feed flows at a high speed within a thermal cracking reactor at $800\text{−}900$ °C with dilution steam. The reactor outlets are mainly ethylene and propylene, as well as olefin, butadiene, and aromatics. The outlet reactor products rapidly cooled down to $300$ °C to prevent unwanted reactions. High-pressure steam was generated using reduced chemistry and post-processing over the CFD fields, proving that realistic predictions can be made in this setting using plant data at the stack.
the resulting energy. Then water and oil were injected to reduce the temperature of the products to virtually room temperature and split up the heavy elements. The pressure of the outlets was then increased to 35 bar. They were sent for fractionation to split up the primary products. 35

Figure 1 is a representation of the process. Thermal cracking reactors are influenced by various performance factors, such as feed composition and feed quantity, reactor pressure and temperature, the amount of the dilution steam, and reactor residence time. The coke precipitate remains on the reactor walls and impairs the furnace’s performance. Monitoring and controlling the optimum factors and parameters enhances the operation and improves the furnace performance.

The reactor resides on the thermal cracking furnace that provides the required heat for the reactions. The inside temperature of the reactor is an essential parameter in thermal cracking reactions due to their endothermic characteristic. Heat flux increasing in the outgoing reactor surface to the highest possible allowed level may expand the amounts of undesirable products such as coke. Therefore, the reactor temperature should be regulated to increase the desired products instead of undesired products. The temperature was increased due to the resident materials in the outlet of the reactor. Nevertheless, the flow should get consistent heat during its process inside the reactor axle. Overheating leads to hot spots and generates local coke. 28

The position of the reactors in thermal cracking furnaces is different. They may be established either in parallel or vertical to the floor regarding the furnace type. Normally, variable-diameter reactors are used as an option for liquid feeds. However, fixed-diameter reactors are used for gassy feeds. The number of reactor paths inside the furnace may vary based on the available technical knowledge.

2.1. Reactor Specifications. The employed reactor is the same as in ref 28 fed by pure propane. Table 1 illustrates the required details.

3. MATHEMATICAL MODEL OF THE THERMAL CRACKING REACTOR

Berreni and Wang prepared an accurate mathematical model of an industrial thermal cracking reactor. Accordingly, the mathematical models were extracted from ref 28. For simplicity, a simple scheme is presented in Figure 2. In addition, other relevant equations were extracted from ref 36.

3.1. Mass Balance Equation. The following equation captures the mass balance for the jth component of the reaction mix along the dz length of the reactor.

\[ \frac{dF_j}{dz} = \frac{R_j \pi d_j^2}{4} = \left( \sum_i \eta_{ji} \right) \frac{\pi d_i^2}{4} \]

where \( r_i \) represents the speed of the ith reaction. The following equation captures \( r_i \):

\[ r_i = K_i \prod \nu_j c_i \]

The molar flow/pressure rate should be considered to apply the speed law. Assuming all the gases as ideal, the general law of gas indicates

\[ c_j = \frac{P_j}{RT} \]

Replacing \( y_j \) (the molar ratio) with its equivalent, \( y_j = \frac{P_j}{n_j} \), leads to

\[ c_j = \frac{F_j P_j}{n_j RT} \]

3.2. Energy Balance Equation. Equation 5 captures the energy balance along the reactor. 28

\[ \frac{dT}{dz} = \sum f_j C_{pj} \left( \nu_{j} \rho_d + \frac{\pi d_j^2}{4} \sum r_i \Delta H_i \right) \]

3.3. Momentum Balance. Equation 6 captures the pressure

\[ \frac{-dP_j}{dz} = \alpha \left( \frac{2f_j}{d_j} + \frac{\xi_j}{\pi n_j} P_j^m \right) \frac{u^2_j}{d_j} + \alpha \frac{u_j}{d_j} \frac{du_j}{dz} \]

The first term on the right-hand side is friction-induced pressure loss. The second term captures the pressure loss induced by momentum change. Regarding the continuity law and the assumption of the gas ideality, the following equations are derived 28

\[ G = p u = \text{const} \]

\[ \rho = \frac{M_m P_t}{RT} \]

\[ u = \frac{G}{M_m} \cdot \frac{RT}{P_t} \]

\[ \frac{du_j}{dz} = \frac{p_t}{P_t} \left[ T \left( \frac{d(1 / M_m)}{dz} + \frac{1}{M_m} \frac{dT}{dz} \right) - \frac{GRT}{M_m P_t^2} \frac{dP}{dz} \right] \]

Substituting the equations gives

Figure 2. Schematic illustration of a thermal cracking reactor. 34

Table 1. Study Reactor’s Specifications 28

| parameter | value |
|-----------|-------|
| length of the coil in the radiant section | 95 [m] |
| length of the straight portion of the coil | 8.85 [m] |
| length of the bends | 0.554 [m] |
| the radius of the bends | 0.178 [m] |
| tube internal diameter | 0.108 [m] |
| wall thickness | 0.008 [m] |
| total feed per coil | 0.7635 [kg/s] |
| steam dilution rate | 0.4 [kg steam/kg propane] |
| inlet pressure | 3 [bar] |
| inlet temperature | 873.15 [K] |
Table 2. Reactions Involved in the Thermal Cracking of Propane$^{37}$

| no | reaction | $A(1/S, m^3/kmol-S or kgS/mol-m)$ | $E$ (kJ/mol) | $\Delta H$ (kJ/mol, @298 K) |
|----|----------|----------------------------------|--------------|-----------------------------|
| 1  | C$_6$H$_6$ $\leftrightarrow$ C$_4$H$_4$ + H$_2$ | $4.692 \times 10^{10}$ | 211.7 | 82.66 |
| 2  | C$_4$H$_8$ $\rightarrow$ C$_4$H$_4$ + H$_2$ | $5.888 \times 10^{10}$ | 214.6 | 124.68 |
| 3  | C$_6$H$_6$ + C$_4$H$_4$ $\rightarrow$ C$_4$H$_4$ + C$_3$H$_6$ | $2.536 \times 10^{13}$ | 241.7 | −11.64 |
| 4  | 2C$_4$H$_8$ $\rightarrow$ 3C$_3$H$_4$ | $1.514 \times 10^{11}$ | 233.5 | 117.5 |
| 5  | 2C$_4$H$_8$ $\rightarrow$ 0.5C$_6$ + 3CH$_4$ | $1.423 \times 10^{9}$ | 190.4 | −14.48 |
| 6  | C$_4$H$_6$ $\leftrightarrow$ CH$_4$ | $3.794 \times 10^{11}$ | 248.5 | 96.4 |
| 7  | C$_2$H$_4$ + C$_2$H$_4$ $\rightarrow$ C$_4$H$_4$ + CH$_4$ | $5.553 \times 10^{14}$ | 251.1 | −11.24 |
| 8  | C$_4$H$_6$ $\rightarrow$ C$_3$H$_4$ + H$_2$ | $4.652 \times 10^{13}$ | 272.8 | 136.32 |
| 9  | C$_4$H$_6$ + CH$_4$ $\rightarrow$ C$_4$H$_4$ + CH$_4$ | $1.026 \times 10^{12}$ | 172.6 | −133.42 |
| 10 | C$_6$H$_6$ $\rightarrow$ C$_6$ | $6.92 \times 10^{7}$ | 143.6 | 83.42 |

For a small element $dz$, we have $\Delta S_p = -\pi D_p(z)/T a(z) dz$. The following illustrates the final entropy generation equation by entropy balance$^{16}$

$$\frac{ds}{dz} = s_{out} - s_{in} - \pi a \int_0^l \frac{J_q(z)}{T_a(z)} dz$$  \hspace{1cm} (22)

Using

$$n = \frac{(F_T / \Omega)RT}{p}$$  \hspace{1cm} (25)

the local entropy generation becomes$^{39}$

$$\sigma = \pi a \int_0^l \frac{J_q(z)}{T_a(z)} dz$$  \hspace{1cm} (24)

Equation 27 shows three facts responsible for entropy in a chemical reactor: the heat transfer to the reactor wall, chemical reactions, and pressure loss. The terms of the above equation result from multiplying thermodynamic flux and its relevant force. The first term includes the multiplication of heat flux $J_q(z)$ and its thermodynamic force $\Delta(1/T)$, the second term includes the multiplication of velocity flux and its thermodynamic force $\left(-\frac{1}{T} \frac{dp}{dz}\right)$, and the last term includes the multiplication of the velocity flux of the reaction $r_i$ and its thermodynamic force $\left(-\frac{\Delta G_i}{T}\right)$.

Integrating $\sigma$ over the reactor length captures the amount of entropy generation as in the following equation

$$\frac{ds}{dz} = \int_0^l \sigma dz$$  \hspace{1cm} (28)

3.5. Entropy Generation in the Thermal Cracking Reactor. The reactor is supposed to function in a stable or steady state. Therefore the entropy balance of the system includes three additional terms. Heat transfer induces two additional entropy factors to the system. So, the following equation captures the amount of entropy generation$^{16}$

$$\frac{ds}{dz} = s_{out} - s_{in} + \Delta s_u$$  \hspace{1cm} (21)

3.6. Kinetic Model Selected for the Research. The molecular mechanism used in this work has been proposed by the authors in ref 37. Propane and water steam were fed into the reactor; they were converted into 12 components throughout 11 reactions. Water steam reactions with other components were
ignored. Table 2 shows these reactions, the activation energy, and the Arrhenius equation factor. Coke formation is ignored in this study. The following equation captures the velocity specific to the reaction $K$, which is a function of temperature:

$$K = A \exp\left(-\frac{E}{RT}\right)$$  \hspace{1cm} (29)

where $A$ is the exponential function coefficient or frequency factor, $E$ is the activation energy (J/mol or cal/mol), $R$ is the ideal gas constant, and $T$ shows the absolute temperature (K).

3.7. Assumptions and Problem-Solving Procedures.

The reactor model is addressed in this section. The pressure, temperature, and weight percent data related to the components and reactor length are used to assess entropy. The reactor simulation assumptions are as follows:

- It is assumed that the internal flow of the reactor is plug flow; because the velocity of the gas is high and the reactor diameter is negligible compared to its length; thus, the axial dispersion of the reactor is ignorable. This assumption is valid based on ref 28.
- Coke deposition is ignored, and the reactor is assumed to be steady-state.

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**Figure 3.** Pseudocode for the MOGA algorithm.

**Figure 4.** (a) Schematic description of the stream’s flow to a specific river and (b) schematic of the WCA optimization process.39
The internal space of the reactor is assumed to be filled only with the combination of gas and steam. The reactions initiate from the input and terminate in the reactor’s output. The input/output hydrodynamic and thermal zone effects are not considered. The concentrations are captured using the law of ideal gas. The relevant equations, i.e., energy, molar, and momentum balance, need to be solved simultaneously. After performing 10 chemical reactions, the feed and pure propane resulted in 10 individual components. Table 2 demonstrates the results. A differential equation is derivable for the components. The molar balance questions are initially equal to zero, except for propane, whose value is given in Table 2. The input feed temperature is required to solve the energy equation, which is a function of the temperature of the outer surface, and its profile is provided based on the length of the reference reactor. Finally, the initial input pressure for the pressure loss equation is known. There are 12 differential equations whose initial conditions are known. They were solved using the MATLAB software package, using the ode15s function, solving complicated differential equations using the GEAR method. Now that all required factors are known, the integral generated in the reactor may be calculated.

### 4. OPTIMIZATION

In this study, two optimization algorithms were used: the multiobjective genetic algorithm (MOGA), a well-known and efficient method for multiobjective optimization, and the multiobjective water cycle algorithm (MOWCA), which is an attractive, recent, and simple concept.

#### 4.1. MOGA.

While GA considered problems with one objective function, MOGAs can overcome this limitation and simultaneously consider two or more objectives. In many industrial problems, objectives under consideration conflict with each other, and optimizing a particular solution related to a single-objective can result in unacceptable results dealing with the other objectives. A reasonable solution to a multiobjective problem is to investigate a set of solutions, each of which satisfies the objectives at an acceptable level without being dominated by any other solution.

Equation 30 mathematically presents a multiobjective optimization problem

\[
\min (f_1(x), f_2(x), ..., f_K(x))
\]

s.t. \(x \in X\)

(30)

where \(K\) is the number of objectives and set \(X\) is the feasible set of decision vectors. The vector-valued objective function can be written as eq 31

\[
f : X \rightarrow \mathbb{R}^K, \quad (f_1(x), f_2(x), ..., f_K(x))^T
\]

(31)

MOGA was used via MATLAB-2020a. The following steps considered the reproductive procedure of the genetic algorithm: natural selection, crossover, mutation, fitness computation,
repair, updation of population, and elitism. While GA is related to one objective function, MOGA can consider more than one objective function. The upper and lower bounds were considered. The MOGA was run in MATLAB software. The pseudocode for the MOGA algorithm used in this study is shown in Figure 3.

4.2. WCA. The water cycle algorithm (WCA) mimics the flow of rivers and streams toward the sea based on the water cycle process. In the case of rain or precipitation, the primary population of design variables (i.e., the population of streams) is randomly increased following the raining process. The best individual variable (i.e., the best stream) with minimum cost function is the sea. Afterward, some good streams with cost function values close to the current best record are assumed as rivers, considering the other remaining streams to have flowed into rivers and the sea. The optimization algorithm should be started with a primary population representing a matrix of streams. For an N-dimensional optimization problem, the following algorithm can be developed using some equations.

\[ N_{sr} = \text{number of Rivers} + 1 \]  \hspace{1cm} (32)

\[ N_{\text{stream}} = N_{\text{pop}} - N_{sr} \]  \hspace{1cm} (33)

where \( N_{\text{pop}} \) and \( N \) represent the total population and the number of design variables, respectively.

\[ NS_n = \text{round}\left(\frac{\text{Cost}_n}{\sum_{i=1}^{N_{sr}} \text{Cost}_i} \times N_{\text{stream}}\right), \text{ } n = 1, 2, \ldots, N_{sr} \]  \hspace{1cm} (34)

where \( NS_n \) is the number of streams that flow to the specific rivers and sea. The following equations may obtain the new position for streams and rivers.

\[ \vec{x}_{\text{Stream}}^{i+1} = \vec{x}_i^{\text{Stream}} + \text{rand} \times C \times (\vec{x}_i^{\text{River}} - \vec{x}_i^{\text{Stream}}) \]  \hspace{1cm} (35)

\[ \vec{x}_{\text{Stream}}^{i+1} = \vec{x}_i^{\text{Stream}} + \text{rand} \times C \times (\vec{x}_i^{\text{Stream}} - \vec{x}_i^{\text{Sea}}) \]  \hspace{1cm} (36)

\[ \vec{x}_{\text{River}}^{i+1} = \vec{x}_i^{\text{River}} + \text{rand} \times C \times (\vec{x}_i^{\text{Sea}} - \vec{x}_i^{\text{River}}) \]  \hspace{1cm} (37)

where \( \text{rand} \) is a uniformly distributed random numbers between 0 and 1. The new position of the streams is determined by

\[ \vec{x}_{\text{Stream}}^{\text{New}} = \vec{x}_{\text{Stream}}^{\text{Old}} + \text{rand} \times (\vec{U} - \vec{L}) \]  \hspace{1cm} (38)

where \( \vec{L} \) and \( \vec{U} \) are lower and upper bounds defined by the given problem, respectively. The value of \( d_{\text{max}} \) adaptively decreases as follows

\[ d_{\text{max}}^{i+1} = d_{\text{max}}^i - d_{\text{max}}^i \frac{\text{Max Iteration}}{\text{Max Iteration}} \]  \hspace{1cm} (39)

Figure 4a shows a schematic view of a stream flowing toward a specific river along their connection line. Figure 4b shows the schematic of the WCA optimization process. Also, Figure 5 shows the flowchart of the water cycle algorithm.

4.3. Optimization Problem. The objective functions of the problem are as follows:

- Maximum production based on weight percentages
- Minimization of entropy generation

Two-objective optimization leads to a two-dimensional Pareto frontier. Thus, the closest solution in the population to the ideal point in the 2D space of the frontier would be considered as the optimum solution to the problem.

The preliminary community should be generated concerning some limitations in the input data, i.e., the constraints of the
decision variables. The values of the constraints are shown in Table 3.

4.4. Genetic Programming. Genetic Programming (GP) generates prediction functions based on decision variables to reduce the optimization run time. In this regard, based on simulation results associated with varying decision variables, the best correlation for estimating objective functions have been proposed by the GP code. Figure 6 shows the algorithm of using GP to generate OFs.

5. RESULTS AND ANALYSIS

5.1. Results for the Reactor in the Reference State. In this research, the main objective was to produce ethylene. The main outputs of the propane thermal cracking reactor included ethylene, methane, propane, propylene, and hydrogen. To verify the computer code for modeling and simulation of the thermal cracking reactor, the simulation results were compared with an industrial case study.28

The percent of propane conversion and the weight of the products were derived by comparing with an industrial reactor. Although coke production was neglected, according to Table 4, the simulation results match the practical results to a high degree of consistency. The weight percent of C3H6 had the highest inconsistency of 12%. The conversion percent difference falls to 0.01%, which was initially the main objective.

Figure 7 illustrates the outer wall temperature profile of the tube, derived from the temperature of the reactor surface in the industrial sample.28

Table 4 presents the results according to the temperature of the outer wall (Figure 8); Figure 8 also depicts the calculation of the governing equations and the temperature profile of the gas mixture. The temperature is 873.15 K at the starting point of the input. As heat is transferred along the tube, the chemical reactions progress, and the outer temperature reaches the wall temperature. Figure 9 depicts the reactor conversion percent, and Figure 10 depicts the weight percent profile of each product.

5.2. Generation of Correlation Using GP. Different simulations were performed to generate the prediction correlations for objective functions with the computer code in the range of decision variables. These data are transferred to the GP code, and the best prediction correlations for objective functions have been achieved, as shown in Table 5. When the mean square error ($R^2$) range is between 0.9 and 1, the accuracy is very high.

The verification of the following equations has been compared with the simulation data with high accuracy. These equations reduce the computation time by about 85%. Also, their accuracy is very high and acceptable.

5.3. Optimization Results. 5.3.1. Multiobjective Optimization. Table 6 presents the Pareto Front optimum solutions for objective functions and decision variables based on MOGA. As shown, the optimum objective functions and corresponding decision variables were determined.

To draw the Pareto front and find the best solution that trade-off between multiple objectives, it is better first to rewrite the target functions in the Pareto optimal solutions so that the difference between the dimensions of the functions is neutralized in the concept of points distance from the ideal point. To make the answers dimensionless, we use the following relation

![Figure 6. Algorithm using GP to generate OFs.](https://doi.org/10.1021/acsomega.1c04345)
OF\_DL\_i,k is the dimensionless objective function for the i-M function and the k-M response, \( i \) is the target function counter, and \( k \) is the response function in that target function. The presentation of the Pareto front for the dimensionless OFs is shown in Figure 11. The 2D normalized Pareto front indicates normalized entropy generation rate versus normalized products. As shown in Figure 11, the point to the coordinates \((1,0)\) is the equilibrium point or ideal point. From the Pareto front’s optimal response set, any response closer to the ideal point is the optimal response. The concept of distance is used according to the following equation to find the closest answer to the ideal point

\[
d_k = \sqrt{(OF_{1,k} - OF_{1,\text{ideal}})^2 + (OF_{2,k} - OF_{2,\text{ideal}})^2}
\]  

(41)

The minimum distance is calculated as 0.5913 and is related to the selected optimal solution, as shown in Table 5.

The optimum values of OFs and decision variables based on MOGA are determined and shown in Table 7. The weight percentage of the basic system products is 60.615%, and the entropy production rate is 1048 J/s. The table above shows that the weighted percentage of products and the system’s entropy production rate after optimization reached 61.13% and 899.8 J/s, displaying an improvement of 0.85 and 16.51%, respectively. The GP and non-GP results also showed similar improvements. However, the computation time of the GP declined significantly (about 85% of the base case).

With MOWCA, the Pareto front optimum solution and its decision variables are indicated in Table 8. The Pareto front optimal solution based on MOWCA is demonstrated in Figure 12. The weight percentage of the products produced in the basic system is 60.61%, and the entropy production rate is 1048 J/s. As shown in Table 9, the weighted percentage of products and the entropy production rate of the system after optimization reached 61.81% and 882.72 J/s, respectively, which resulted in an improvement of 1.97 and 18.77%, respectively. As shown in Table 9, the optimization with GP and non-GP algorithms shows similar results.

5.3.2. Single-Objective Optimization. In this case, two optimization processes are implemented with one of the target functions. Optimization results to maximize product production lead to 64.36% by weight of system products, equivalent to a 6.17% increase in product production. The single-objective optimization response aims to maximize product production, as shown in Table 10.
Table 5. Objective Function Correlation Generated by GP

| Objective | Best Equation | Mean Square Error |
|-----------|---------------|------------------|
| Products (%) | $0.00127 \times P_{\text{gas}} + 7045.399 \times \log(T_a) + 1.55E-28 \times P_{\text{gas}} \times T_a^2 - 42402.84 \times T_a - 1.38E - 9 \times P_{\text{gas}} \times T_a^2$ | 0.97 |
| Entropy Generation | $+ 1.498 \times \frac{\tau_g}{\tau_{P_{\text{gas}}} \times \tau_{T_a}} - 1.60E17 \times \frac{\tau_g}{\tau_{P_{\text{gas}}} \times \tau_{T_a}}$ | 0.94 |

Table 6. Pareto front optimum solutions for Objective Functions Based on MOGA

| OF1 | OF2 | DV1 | DV2 | DV3 | DV4 |
|-----|-----|-----|-----|-----|-----|
| products (J/K s) | entropy (J/K s) | $T_{\text{gas,in}}$ (K) | $P_{\text{gas,in}}$ (kPa) | $m_a$ (g/s) | $T_{w,in}$ (K) |
| 44.19 | 699.63 | 852.71 | 250.002 | 750.00 | 1000.00 |
| 44.19 | 699.63 | 852.71 | 250.002 | 750.00 | 1000.00 |
| 48.41 | 741.06 | 853.11 | 250.003 | 750.76 | 1010.39 |
| 64.45 | 986.14 | 852.79 | 250.004 | 751.05 | 1098.55 |
| 54.50 | 807.46 | 852.88 | 250.004 | 750.30 | 1028.40 |
| 56.42 | 831.17 | 853.15 | 250.004 | 750.40 | 1035.97 |
| 55.44 | 818.78 | 852.99 | 250.003 | 750.22 | 1032.20 |
| 46.07 | 717.76 | 852.91 | 250.003 | 750.53 | 1004.44 |
| 52.80 | 787.75 | 852.97 | 250.003 | 750.25 | 1023.12 |
| 64.17 | 971.10 | 853.49 | 250.005 | 750.43 | 1090.57 |
| 60.10 | 882.90 | 853.03 | 250.004 | 750.45 | 1053.11 |
| 61.61 | 908.49 | 852.94 | 250.004 | 750.22 | 1062.63 |
| 51.84 | 777.23 | 853.31 | 250.004 | 750.73 | 1020.13 |
| 57.14 | 840.46 | 853.07 | 250.004 | 750.43 | 1038.88 |
| 63.39 | 946.53 | 853.34 | 250.004 | 750.45 | 1078.57 |
| 45.68 | 713.97 | 852.83 | 250.003 | 750.39 | 1003.51 |
| 63.15 | 940.32 | 853.40 | 250.005 | 750.39 | 1075.81 |
| 46.94 | 726.23 | 853.01 | 250.003 | 750.42 | 1006.60 |
| 61.29 | 902.59 | 853.46 | 250.004 | 750.32 | 1060.42 |
| 57.84 | 849.82 | 853.28 | 250.003 | 750.53 | 1041.89 |
| 58.72 | 862.21 | 852.95 | 250.002 | 750.40 | 1045.97 |
| 63.64 | 953.19 | 853.46 | 250.004 | 750.35 | 1081.70 |
| 62.87 | 933.99 | 853.27 | 250.002 | 750.60 | 1073.00 |
| 53.02 | 790.38 | 852.96 | 250.004 | 750.40 | 1023.85 |
| 59.33 | 871.11 | 852.94 | 250.004 | 750.44 | 1048.98 |
| 64.04 | 966.05 | 853.28 | 250.004 | 750.43 | 1087.93 |
| 64.56 | 1001.43 | 853.54 | 250.005 | 751.93 | 1108.04 |
| 52.43 | 783.61 | 852.97 | 250.004 | 750.22 | 1021.96 |
| 49.20 | 748.99 | 852.76 | 250.003 | 750.16 | 1012.52 |
| 45.08 | 708.22 | 852.06 | 250.003 | 750.46 | 1002.08 |
| 53.46 | 795.40 | 852.93 | 250.003 | 750.42 | 1025.28 |
| 61.13 | 899.80 | 853.42 | 250.004 | 750.36 | 1059.36 |
| 46.98 | 726.65 | 852.95 | 250.004 | 750.40 | 1006.71 |
| 44.44 | 701.94 | 852.72 | 250.002 | 750.02 | 1000.56 |
| 60.60 | 891.09 | 852.76 | 250.003 | 750.39 | 1056.04 |
| 50.23 | 759.82 | 853.21 | 250.003 | 750.57 | 1015.38 |
| 58.08 | 853.21 | 853.17 | 250.003 | 750.41 | 1043.00 |
| 62.45 | 974.33 | 853.52 | 250.004 | 750.42 | 1092.29 |
| 60.58 | 890.60 | 853.27 | 250.003 | 750.43 | 1055.92 |
| 54.33 | 805.38 | 853.09 | 250.004 | 750.24 | 1028.21 |
| 54.96 | 813.05 | 853.28 | 250.003 | 750.40 | 1030.44 |
| 55.77 | 823.00 | 852.72 | 250.004 | 750.20 | 1033.46 |
| 61.95 | 914.86 | 853.22 | 250.003 | 750.54 | 1065.11 |
| 62.68 | 929.68 | 852.97 | 250.004 | 750.37 | 1071.16 |
| 56.08 | 826.87 | 853.29 | 250.003 | 750.68 | 1034.62 |
| 64.55 | 996.99 | 853.48 | 250.005 | 751.88 | 1105.13 |
| 47.57 | 732.49 | 852.80 | 250.003 | 750.27 | 1008.21 |
| 62.39 | 923.42 | 853.46 | 250.005 | 750.37 | 1068.63 |

The optimization results aimed at minimizing the entropy production rate lead to the production of 687.99 (J/K s) entropy in the system, equivalent to a decrease of 52.38% in the production of the entropy production rate of the system. The solution to the single-objective optimization to minimize the entropy production of the system is indicated in Table 11. Also, a single optimization using WCA has been performed. The optimization results aim to maximize the product, leading to the formation of 64.56% by weight of product, equivalent to a 6.51% increase in product production as determined in Table 12. The optimization results aimed at minimizing the entropy production rate lead to the production of 687.50 (J/K s) entropy...
in the system, equivalent to a decrease of 52.49% in the production of the entropy production rate of the system, as shown in Table 13.

5.4. Computational Time. The computational time for MOGA, MOWCA, GP-MOGA, and GP-MOWCA are indicated in Table 14. In the GP-MOGA and GP-MOWCA, the time for generation of data sets and GP correlations have been considered.

Table 8. Pareto Front Optimum Solutions for Objective Functions Based on MOWCA

| OF1 products (%) | OF2 entropy generation (J/K s) | DV1 $T_{gas,in}$ (K) | DV2 $P_{gas,in}$ (bar) | DV3 $m_a$ (g/s) | DV4 $T_{w,in}$ (K) |
|-----------------|-------------------------------|---------------------|-----------------------|----------------|------------------|
| 64.56 | 962.27 | 943.15 | 250.00 | 750.00 | 1108.01 |
| 44.19 | 689.91 | 943.15 | 250.00 | 750.00 | 1000.00 |
| 44.19 | 689.91 | 895.34 | 309.530 | 816.06 | 1119.54 |
| 64.56 | 962.27 | 943.15 | 250.00 | 750.00 | 1108.01 |
| 63.37 | 912.68 | 943.15 | 250.00 | 750.00 | 1078.33 |
| 62.08 | 886.71 | 943.15 | 250.00 | 750.00 | 1066.12 |
| 48.95 | 733.39 | 943.15 | 250.00 | 753.29 | 1101.83 |
| 45.71 | 702.98 | 943.15 | 250.00 | 750.00 | 1003.58 |
| 44.78 | 694.93 | 943.15 | 250.00 | 750.00 | 1001.36 |

Table 9. Pareto Front Optimum Solutions for Objective Functions Based on MOWCA

| optimum objective function parameters | products (normalized) | entropy generation (normalized) | products (%) | entropy generation (J/K s) |
|---------------------------------------|-----------------------|---------------------------------|--------------|--------------------------|
| with GP value                         | 0.86                  | 0.71                            | 61.81        | 882.72                   |
| without GP value                      | 0.86                  | 0.71                            | 61.81        | 882.72                   |

Table 10. Results of Maximization of the Product by GA

| optimum objective function parameters | products (%) | entropy generation (J/K s) |
|---------------------------------------|--------------|--------------------------|
| with GP value                         | 64.36        | 1022.20                  |
| without GP value                      | 64.36        | 1022.20                  |

Figure 12. Normalized Pareto front optimum solution obtained with MOWCA.

Table 11. Results of Minimization of Entropy Generation by GA

| optimum objective function parameters | products (%) | entropy generation (J/K s) |
|---------------------------------------|--------------|--------------------------|
| with GP value                         | 48.92        | 688.00                   |
| without GP value                      | 48.92        | 688.00                   |

The computation time is based on Intel Core i7-8750H with 6 CPU cores and 16 GB memory. As seen, the computation time is
were obtained:

- Temperature, inlet gas pressure, the mass and WCA were performed to maximize products and minimize the governing equations was investigated.

- The amount of entropy generated by the sources and products were propane, methane, ethylene, propylene, and hydrogen. The input feed was propane and water steam, and the main output was the weighted percentage of products and the entropy generation rate of the system. WCA led to a decrease of 52.38 and 52.49% compared to the base case.

- The base case in the entropy generation rate of the system. WCA led to a decrease of 52.38 and 52.49% compared to the base case in the entropy generation rate of the system. WCA led to a decrease of 52.38 and 52.49% compared to the base case.

- The authors declare no competing financial interest.

### 6. CONCLUSIONS

A thermal cracking reactor was investigated in this study. The input feed was propane and water steam, and the main output products were propane, methane, ethylene, propylene, and hydrogen. The amount of entropy generated by the sources and the governing equations was investigated.

Single-objective and two-objective optimizations using GA and WCA were performed to maximize products and minimize entropy generation. Decision variables were the inlet gas temperature, inlet gas pressure, the mass flow rate of the inlet air, and the wall. GP was employed to generate the best correlations to predict objective functions based on key variables to reduce the run time of optimization runs.

Based on single-objective optimization, the following results were obtained:

- Maximizing product production using GA and WCA led to 64.36 and 64.56% by weight of system products equivalent to a 6.17 and 6.51% increase in the product compared to the base case.

- Minimizing the entropy production rate using the GA and WCA led to a decrease of 52.38 and 52.49% compared to the base case in the entropy generation rate of the system.

Based on two-objective optimization, the following results were obtained:

- The weighted percentage of products and the entropy production rate improved 0.85% and 16.51% compared with the base case using the MOGA algorithm, and 1.97 and 18.77% compared to the base case.

It is suggested that future studies will address exergonic and exergoeconomic parameters. For studies on the optimization problem, environmental impacts are critical factors that should be further investigated.

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### Notes

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### NOMENCLATURE

- $j$: $j$th component
- $dz$: the length $dz$
- $F_j$: the intensity of the molar flow of the $j$th component
- $a_{ij}$: stoichiometric coefficient of the $j$th component in the $i$th reaction
- $R_i$: overall velocity of the production and/or consumption of the $j$th component
- $r_i$: the velocity of the $i$th reaction
- $K_i$: the specific velocity of the $i$th reaction
- $c_j$: the molar concentration of the $j$th component
- $y_j$: molar ratio
- $\Delta H_i$: the heat of the $i$th reaction
- $J_\alpha(z)$: heat flux transferred from the outer heat source to the reaction flow in the location $z$ of the reactor
- $C_p$: heat capacity of the $j$th component
- $\alpha$: unit conversion factor
- $\rho$: gas density
- $u$: gas speed
- $M_m$: gas mixture molecular weight
- $A$: the angle of the bends, which is equal to 180°
- $T_w$: surface temperature
- $T_\infty$: fluid temperature
- $h$: the coefficient of the convection heat transfer
- $T_c$: the temperature of the tube center
- $T_b$: bulk temperature
- $T_{bo}$: outlet bulk temperature
- $S_m$: entropy of the inlet flow
- $S_{out}$: entropy of the outlet flow
- $\Delta S_n$: entropy induced by heat transfer

| Table 12. Results of Maximization of the Product by WCA |
|---|---|---|
| optimum objective function parameters | with GP value | without GP value |
| products (%) | 64.36 | 64.56 |
| entropy generation (J/K s) | 1099.20 | 1099.20 |
| optimum decision variables parameters | with GP value | without GP value |
| $T_{gas, in}$ (K) | 915.27 | 915.27 |
| $P_{gas, in}$ (bar) | 35.39 | 35.39 |
| $m_i$ (g/s) | 25 | 25 |
| $T_{w, in}$ (K) | 1108.01 | 1108.01 |

| Table 13. Results of Minimization of Entropy Generation by WCA |
|---|---|---|
| optimum objective function parameters | with GP value | without GP value |
| products (%) | 59.66 | 59.66 |
| entropy generation (J/K s) | 687.50 | 687.50 |
| optimum decision variables parameters | with GP value | without GP value |
| $T_{gas, in}$ (K) | 878.08 | 878.08 |
| $P_{gas, in}$ (bar) | 28.03 | 28.03 |
| $m_i$ (g/s) | 799.67 | 799.67 |
| $T_{w, in}$ (K) | 1161.73 | 1161.73 |

| Table 14. Comparison of Computation time for MOGA, MOWCA, GP-MOGA, and GP-MOWCA |
|---|---|---|---|
| methodology | MOGA | MOWCA | GP-MOGA | GP-MOWCA |
| computation time (s) | 63 056.8 | 61 753 | 34 270 | 33 380 |
| computation time (h) | 17.51 | 17.15 | 9.52 | 9.27 |

Reduced significantly in GP-MOWCA and GP-MOGA compared with MOGA and MOWCA.40
\[ \sigma \quad \text{locally generated entropy} \]
\[ \text{coefficient of exponential function or coefficient of frequency} \]
\[ E \quad \text{the activation energy (expressed in J/mol or cal/mol)} \]
\[ R \quad \text{ideal gas constant} \]
\[ T \quad \text{absolute temperature, K} \]

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