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Development and Validation of a Pyrolyzer Model for Ethylene Production from Natural Gas Liquids Using Mass and Energy Balance Approaches

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Abstract
Ethylene is one of the most important petrochemical feedstocks used in the production of plastics, synthetic fibers, solvents, and numerous industrial chemicals. The increasing global demand for ethylene has necessitated the development of efficient and sustainable production technologies. Natural gas liquids (NGLs), particularly ethane, have emerged as attractive feedstocks for ethylene production because of their high hydrogen-to-carbon ratio, availability, and favorable cracking characteristics. This study developed a pyrolyzer model for ethylene production from natural gas liquids using fundamental mass and energy balance approaches. The model was implemented in MATLAB to simulate the performance of a tubular pyrolysis reactor under varying operating conditions. Reactor performance was evaluated using fractional conversion, reactor temperature, reactor volume, pressure drop, space time, and space velocity as key performance indicators. The simulation results showed that reactor temperature increased from 894 K to 1063 K as conversion increased from 10% to 90%, while reactor volume, pressure drop, and space time exhibited corresponding increases. Conversely, space velocity decreased with increasing conversion due to longer residence time requirements. Model validation was conducted through comparison with published benchmark literature data. The validation results showed prediction deviations below 5% for major reactor performance parameters, indicating good agreement between model outputs and reported industrial operating conditions. The developed model provides a reliable preliminary engineering tool for pyrolysis reactor analysis, process evaluation, and future optimization studies involving ethylene production from natural gas liquids.

Keywords: *Ethylene production, Mass balance, Natural gas liquids, Pyrolysis reactor, Reactor modelling, Validation*

I. INTRODUCTION

Ethylene is one of the most extensively produced organic chemicals in the global petrochemical industry and serves as a fundamental building block for numerous industrial products, including polyethylene, polyvinyl chloride, ethylene oxide, ethylene glycol, styrene, and various specialty chemicals (Khan et al., 2022). The growing global demand for plastics, packaging materials, synthetic fibers, and chemical intermediates has resulted in a continuous increase in ethylene consumption worldwide. According to the International Energy Agency (2023), petrochemical production accounts for a significant proportion of global industrial growth, with ethylene remaining one of the most commercially important products in the sector.

Conventionally, ethylene is produced through thermal cracking processes involving hydrocarbon feedstocks such as naphtha, liquefied petroleum gas (LPG), and natural gas liquids (NGLs). Among these feedstocks, natural gas liquids have gained considerable attention due to their abundant availability, lower carbon intensity, favorable economics, and high ethylene yield

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potential (Faramawy et al., 2016). Ethane-rich NGL streams are particularly attractive because they produce higher ethylene selectivity and fewer undesirable by-products compared with heavier hydrocarbon feedstocks (Saeed et al., 2021). The primary industrial method for ethylene production is steam cracking or pyrolysis, where hydrocarbon feedstocks are subjected to elevated temperatures, typically between 800 K and 1200 K, in the presence of steam and under controlled residence times (Towfighi et al., 2020). During pyrolysis, hydrocarbon molecules undergo thermal decomposition, producing lighter olefins, particularly ethylene. The efficiency of this process is influenced by several operational variables, including temperature, pressure, residence time, feed composition, and reactor configuration (Treger & Rozhkov, 2016).

Because industrial pyrolysis reactors operate under highly demanding thermal and kinetic conditions, mathematical modelling has become an essential tool for reactor design, optimization, and performance evaluation. Mathematical models enable engineers to predict reactor behavior under different operating conditions, evaluate process performance, reduce experimental costs, and support decision-making during process development (Fogler, 2021). Among the various modelling approaches available, mass and energy balance techniques remain fundamental because they provide a systematic framework for describing material transformations and energy interactions within chemical reactors (Levenspiel, 2019).

Several researchers have investigated the modelling and optimization of pyrolysis systems for olefin production. Qyyum et al. (2022) developed simulation-based approaches for sustainable ethylene production from natural gas liquids and demonstrated the importance of process optimization in improving product yield and energy efficiency. Sundaram et al. (2022) presented a mathematical model for thermal cracking reactors and reported the influence of operating conditions on reactor performance. Similarly, Hussain et al. (2023) developed optimization frameworks for hydrocarbon pyrolysis reactors and highlighted the significance of temperature control and residence time in maximizing olefin production. Zhao et al. (2023) further emphasized the role of simulation and modelling techniques in enhancing the efficiency of ethylene production systems.

Despite these advancements, many existing studies rely on highly detailed kinetic mechanisms involving numerous reaction pathways, extensive computational resources, and proprietary industrial datasets. Such models are often difficult to reproduce and may not be suitable for preliminary engineering design applications. Furthermore, some published studies focus primarily on simulation outputs without providing transparent mathematical formulations that can easily be adapted for educational and engineering purposes. Consequently, there remains a need for a simplified, transparent, and reproducible pyrolyzer model that utilizes fundamental mass

and energy balance principles while still providing reliable engineering predictions. Such a model can serve as a valuable tool for preliminary reactor analysis, performance evaluation, and educational applications.

This study addresses this gap by developing a MATLAB-based pyrolyzer model for ethylene production from natural gas liquids using mass and energy balance approaches. The model evaluates key reactor performance indicators, including fractional conversion, reactor temperature, reactor volume, pressure drop, space time, and space velocity. Unlike previous studies that rely heavily on complex kinetic networks, the present work adopts a simplified engineering modelling framework and validates the resulting predictions against published benchmark literature data. The primary objective of this study is therefore to develop and validate a pyrolyzer model for ethylene production from natural gas liquids using mass and energy balance principles and to evaluate reactor performance under varying conversion conditions.

The findings are expected to contribute to reactor modelling research and provide a useful engineering tool for preliminary process analysis and future optimization studies. The remainder of this paper is organized as follows. Section II presents the literature review related to natural gas liquids, ethylene production, pyrolysis reactor modelling, and model validation. Section III describes the research methodology, including model development, assumptions, governing equations, simulation procedures, and validation methods. Section IV presents the results and discussion of the simulation outcomes and validation analysis. Finally, Section V summarizes the major findings, limitations, and recommendations for future research.

II. LITERATURE REVIEW

A. Natural Gas Liquids and Ethylene Production

Natural gas liquids (NGLs) are hydrocarbon components recovered from natural gas streams during gas processing operations. They primarily consist of ethane, propane, butane, isobutane, and natural gasoline. The increasing availability of shale gas resources and associated natural gas production has significantly expanded the global supply of NGLs, making them attractive feedstocks for petrochemical manufacturing (Faramawy et al., 2016). Among the various NGL components, ethane is considered one of the most desirable feedstocks for ethylene production because of its high hydrogen-to-carbon ratio and relatively simple molecular structure. Ethane cracking generally produces higher ethylene yields and fewer by-products than heavier hydrocarbon feedstocks such as naphtha (Khan et al., 2022). The growing adoption of ethane-based cracking technologies has contributed significantly to improvements in process efficiency and reductions in greenhouse gas emissions associated with petrochemical production.

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Ethylene occupies a central position within the petrochemical value chain due to its extensive use in the manufacture of plastics, solvents, synthetic fibers, antifreeze compounds, and chemical intermediates. According to the International Energy Agency (2023), ethylene demand is expected to continue increasing due to expanding industrialization, urbanization, and consumer product manufacturing worldwide. Consequently, improvements in ethylene production technologies remain an important area of research and industrial development. The selection of feedstock significantly influences reactor performance, product yield, energy consumption, and overall process economics. Studies by Saeed et al. (2021) demonstrated that variations in feedstock composition can substantially affect olefin yield and cracking efficiency. Therefore, understanding the characteristics of NGL feedstocks is essential for developing reliable reactor models and optimizing ethylene production systems.

B. Pyrolysis and Steam Cracking Technology

Pyrolysis, commonly referred to as steam cracking in industrial applications, is the dominant technology used for large-scale ethylene production. The process involves the thermal decomposition of hydrocarbons at elevated temperatures, typically between 800 K and 1200 K, under carefully controlled operating conditions (Towfighi et al., 2020). During pyrolysis, hydrocarbon molecules absorb thermal energy and undergo bond cleavage, generating smaller hydrocarbon fragments and olefin products. For ethane feedstocks, the primary reaction can be represented as: $C_2H_6 \rightarrow C_2H_4 + H_2$. This reaction is highly endothermic and requires substantial heat input to maintain reactor operation. The performance of a pyrolysis reactor depends on several key parameters, including reactor temperature, residence time, feed composition, pressure, and heat transfer characteristics (Treger & Rozhkov, 2016).

Temperature is widely recognized as one of the most influential variables affecting cracking performance. Higher temperatures generally increase reaction rates and conversion levels; however, excessively high temperatures may promote secondary cracking reactions, coke formation, and undesirable by-product generation (Demirbas, 2021). Similarly, residence time influences the extent of feed conversion and product selectivity. Longer residence times often improve conversion but may also increase secondary reactions and reduce product quality. Recent studies have emphasized the need for improved reactor designs and optimized operating conditions to maximize ethylene yield while minimizing energy consumption and operational costs (Ranjan et al., 2023). Consequently, accurate reactor modelling has become an essential component of modern pyrolysis process development.

C. Pyrolysis Reactor Modelling

Mathematical modelling provides a powerful approach for analyzing reactor behaviour, predicting process performance, and supporting engineering design decisions. Reactor models allow engineers to evaluate different operating conditions without conducting expensive and time-consuming experimental investigations (Fogler, 2021). Several modelling approaches have been applied to pyrolysis reactors, including kinetic models, computational fluid dynamics (CFD) simulations, process simulators, and mass-energy balance models. Kinetic models typically incorporate detailed reaction mechanisms involving multiple reaction pathways and intermediate species. While such models can provide highly accurate predictions, they often require extensive computational resources and detailed reaction data (Sundaram et al., 2022).

Process simulation tools have also been widely used for evaluating ethylene production systems. Qyyum et al. (2022) employed process simulation and optimization techniques to investigate sustainable ethylene production from natural gas liquids. Their study demonstrated that simulation-based approaches can significantly improve process performance and energy efficiency. Similarly, Hussain et al. (2023) developed optimization models for hydrocarbon pyrolysis reactors and reported strong relationships between reactor temperature, residence time, and olefin production efficiency. Zhao et al. (2023) further highlighted the importance of simulation techniques in improving reactor design and operational performance. Although advanced simulation models offer high predictive capability, many are difficult to reproduce because they rely on proprietary industrial data or highly complex reaction networks. As a result, simplified engineering models based on fundamental mass and energy balances remain valuable tools for preliminary reactor design and educational applications.

D. Mass and Energy Balance Applications in Reactor Design

Mass and energy balance principles constitute the foundation of chemical reactor analysis and design. These principles are based on the conservation of mass and energy and provide a systematic framework for describing material and thermal transformations within engineering systems (Levenspiel, 2019). Mass balance equations are used to quantify the consumption of reactants and formation of products throughout the reactor. In pyrolysis systems, mass balances enable the determination of conversion levels, product yields, and flow-rate variations. Energy balance equations describe heat transfer and thermal interactions within the reactor and are essential for predicting temperature profiles and heat requirements (Smith et al., 2021). The combined application of mass and energy balances has been widely utilized in chemical reactor design, process simulation, and performance evaluation. According to Ghasem (2022), mass-energy balance models provide reliable engineering predictions while maintaining mathematical simplicity and computational efficiency. For pyrolysis reactors, mass and energy balance methods

are particularly useful because they allow engineers to estimate reactor performance under varying operating conditions and support preliminary design decisions. These models are frequently used during conceptual design stages before more detailed kinetic or computational analyses are undertaken.

E. Model Validation in Chemical Reactor Studies

Model validation is a critical component of engineering modelling because it establishes confidence in the reliability and predictive capability of simulation results. Validation involves comparing model outputs against experimental observations, industrial operating data, published benchmark values, or previously validated models (Montgomery & Runger, 2020). In chemical reactor modelling studies, validation ensures that mathematical formulations adequately represent actual process behaviour. Without validation, simulation results cannot be considered reliable for engineering analysis or decision-making purposes. Researchers commonly assess validation performance using percentage error analysis, statistical indicators, or comparative evaluations with literature data.

Sundaram et al. (2022) validated their thermal cracking reactor model using published experimental data and reported good agreement between predicted and observed conversion values. Similarly, Qyyum et al. (2022) compared simulation outputs with benchmark process data to evaluate the reliability of their ethylene production model. Such approaches have become widely accepted in preliminary engineering studies where direct industrial operating data may not be readily available. Validation is particularly important for reactor performance parameters such as temperature, conversion, residence time, and pressure drop because these variables directly influence reactor efficiency and operational effectiveness. Therefore, incorporating validation procedures into reactor modelling studies enhances the credibility and practical relevance of the developed models.

F. Research Gap

Although numerous studies have investigated hydrocarbon pyrolysis and ethylene production using advanced kinetic models, process simulators, and optimization frameworks, many of these approaches depend on extensive reaction mechanisms, large computational requirements, and proprietary industrial datasets. Such complexities often limit their accessibility, reproducibility, and usefulness for preliminary engineering design applications. Existing studies frequently employ detailed kinetic mechanisms and proprietary datasets that limit reproducibility. This study contributes a simplified and transparent modelling framework that can be readily reproduced using standard engineering principles. Furthermore, several published studies focus primarily on

simulation outputs without presenting transparent mathematical formulations based on fundamental engineering principles.

Consequently, there remains a need for a simplified, reproducible, and computationally efficient modelling framework that integrates mass and energy balance concepts while maintaining acceptable predictive accuracy. This study addresses this gap by developing a MATLAB-based pyrolyzer model for ethylene production from natural gas liquids using mass and energy balance approaches. Unlike many existing models, the proposed framework emphasizes simplicity, transparency, reproducibility, and validation against published benchmark literature data while still providing meaningful engineering predictions for reactor performance analysis.

III. RESEARCH METHOD(S)

A. Research Design

This study employed a quantitative modelling and simulation approach for the development of a pyrolyzer model aimed at ethylene production from natural gas liquids (NGLs). The modelling framework was developed based on fundamental principles of chemical reaction engineering, incorporating mass balance, energy balance, reaction kinetics, and reactor design equations. The model was implemented using MATLAB R2024a to simulate reactor performance under varying operating conditions.

Table 1. Nomenclature of Model Variables

Symbol	Description	Unit
X	Fractional conversion	–
V	Reactor volume	m^3
T	Reactor temperature	K
P	Pressure	kPa
ΔP	Pressure drop	kPa
τ	Space time	s
SV	Space velocity	s^{-1}
F_{ao}	Initial molar flow rate of reactant	mol/s
F_a	Molar flow rate of reactant at any point	mol/s
C_a	Reactant concentration	mol/m^3
r_a	Reaction rate	$mol/m^3 \cdot s$
k	Reaction rate constant	s^{-1}
E_a	Activation energy	kJ/mol
R	Universal gas constant	kJ/mol·K
Cp	Heat capacity	kJ/kg·K
Q	Heat supplied to the reactor	kJ
ρ	Density	kg/m^3

The developed model was designed to evaluate the influence of key process variables on reactor performance, including fractional conversion, reactor temperature, reactor volume, pressure drop, space time, and space velocity. A tubular pyrolysis reactor operating under steady-state conditions was considered as the reactor configuration. Mathematical relationships governing mass conservation, energy conservation, reaction kinetics, and fluid flow were integrated into a

computational framework to predict reactor behaviour and assess process efficiency. The symbols and parameters utilized throughout this study are presented in Table 1.

B. *Feedstock Description*

The feedstock considered in this study was an ethane-rich natural gas liquid stream. Ethane was selected as the primary feed component because it is widely used in industrial steam-cracking processes for ethylene production due to its high conversion efficiency and favourable product selectivity (Khan et al., 2022). The feedstock considered in this study was an ethane-rich natural gas liquid stream. Ethane was selected as the primary feed component because it is widely used in industrial steam-cracking processes for ethylene production due to its high conversion efficiency and favourable product selectivity (Khan et al., 2022).

Table 2. Representative Feed Composition

Component	Composition (%)
Ethane (C_2H_6)	90
Propane (C_3H_8)	5
Butane (C_4H_{10})	3
Other Hydrocarbons	2

C. Model Assumptions

To simplify the mathematical formulation and facilitate computational implementation, the following assumptions were adopted:

1. Reactor operation occurs under steady-state conditions.
2. The reactor behaves as a plug flow reactor (PFR).
3. Ideal gas behaviour is assumed throughout the reactor.
4. Heat losses to the surroundings are negligible.
5. Radial temperature gradients are neglected.
6. The reaction mixture is perfectly mixed in the radial direction.
7. Ethane cracking represents the dominant reaction pathway.
8. Catalyst effects are neglected because thermal pyrolysis is considered.
9. Physical properties remain approximately constant within the operating range.
10. Coke formation and secondary cracking reactions are not explicitly modelled.

These assumptions are consistent with preliminary reactor modelling studies reported in the literature (Fogler, 2021; Levenspiel, 2019).

D. *Scheme and Kinetic Model*

The primary pyrolysis reaction considered in this study is the thermal cracking of ethane to produce ethylene and hydrogen using.

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

The reaction was assumed to follow first-order kinetics with respect to ethane concentration. The rate expression is given by:

$$-r_A = kC_A$$

where, r_A for reaction rate (mol/m^{-3} s^{-1}), k for reaction rate constant (s^{-1}), and C_A for ethane concentration (mol/m^{-3}). The temperature dependence of the rate constant was described using the Arrhenius equation:

$$k = Ae^{-E_a/RT}$$

where A for frequency factor, Ea for activation energy (kJ/mol^{-1}), R for universal gas constant, and T denotes absolute temperature (K).

E. *Mass Balance Formulation*

For a plug flow reactor operating under steady-state conditions, the differential mole balance is expressed as:

$$\frac{dF_A}{dV} = r_A$$

Substituting the first-order reaction expression:

$$\frac{dF_A}{dV} = -kC_A$$

The fractional conversion is defined as:

$$X = \frac{F_{A0} - F_A}{F_{A0}}$$

Rearranging the reactor design equation gives:

$$V = \int_0^X \frac{F_{A0}}{-r_A} dX$$

This equation was used to determine reactor volume requirements at different conversion levels.

F. *Energy Balance Formulation*

The pyrolysis process is highly endothermic and therefore requires continuous heat input. The general steady-state energy balance for the reactor is:

$$Q + F_{in} H_{in} = F_{out} H_{out}$$

The temperature rise within the reactor was estimated using:

$$Q = mC_p(T_2 - T_1)$$

where, Q for heat supplied, m is for mass flow rate, C_p for heat capacity, T_1 for inlet temperature, and T_2 for outlet temperature. The energy balance was incorporated into the MATLAB program to determine reactor temperature profiles corresponding to various conversion level.

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G. Pressure Dropp Model

Pressure losses occurring along the reactor length were estimated using a simplified pressure-drop relationship:

$$\Delta P = f \frac{L}{D} \frac{\rho u^2}{2}$$

where, f for friction factor, L for reactor length, D for reactor diameter, ρ for fluid density, and u for superficial velocity. Pressure drop was evaluated as a function of reactor operating conditions and conversion levels.

H. Space Time and Space Velocity Analysis

Space time represents the average residence time required for the feed to pass through the reactor. The space time relationship is expressed as:

$$r = \frac{V}{v_0}$$

where, r for space time (s), V for reactor volume (m^3), V_0 for volumetric feed rate ($m^3\ s^{-1}$).
Space velocity was calculated using:

$$SV = \frac{1}{r}$$

Space time and space velocity provide useful indicators of reactor productivity and operational performance.

I. Boundary Conditions and Operator Parameters

The simulation was conducted under the operating conditions presented in Table 3.

Table 3. Simulation Boundary Conditions

Parameter	Value
Feed temperature	850 K
Maximum reactor temperature	1100 K
Feed pressure	200 kPa
Conversion range	10–90%
Feed flow rate	100 mol/s
Reactor diameter	0.50 m
Reactor length	5.0 m

The selected conditions are consistent with industrial ethylene pyrolysis operations reported in previous studies (Towfighi et al., 2020).

J. MATLAB Simulation Procedure

The mathematical equations developed in this study were implemented using MATLAB R2024a. The computational procedure involved:

1. Input of feedstock composition and operating conditions.
2. Ideal gas behaviour is assumed throughout the reactor.
3. Calculation of reaction kinetics using Arrhenius relationships.

4. Evaluation of mass balance equations.
5. Evaluation of energy balance equations.
6. Determination of reactor volume requirements.
7. Calculation of pressure drop.
8. Calculation of space time and space velocity.
9. Generation of graphical outputs.
10. Comparison of results with benchmark literature data.

The simulation outputs were generated over a conversion range of 10%–90%.

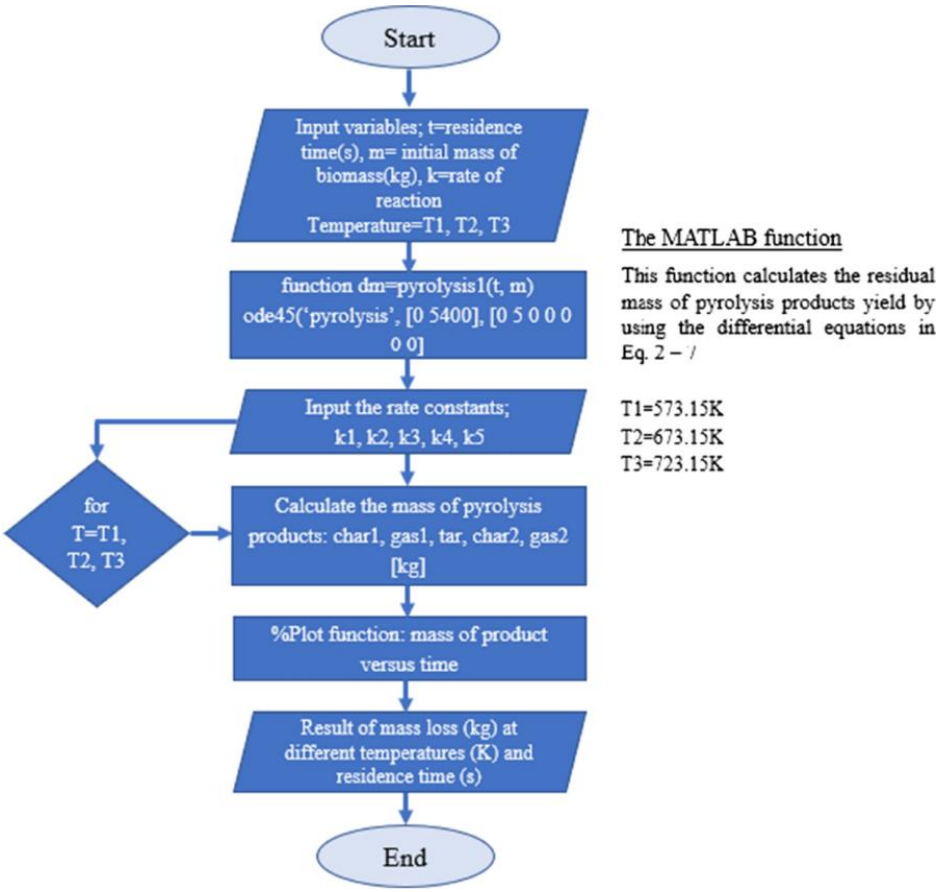

Figure 1. Methodological framework

K. Model Validation Procedure

Model validation was performed by comparing simulation outputs with published benchmark literature data obtained from previous ethylene pyrolysis studies (Qyyum et al., 2022; Sundaram et al., 2022; Hussain et al., 2023). Validation was conducted using percentage error analysis:

$$\%\ Error = \left|\frac{Experimental - Model}{Experimental}\right| \text{ x } 100$$

The parameters selected for validation included:

- Reactor temperature

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- Fractional conversion
- Space time
- Pressure drop

Prediction errors below 5% were considered indicative of acceptable model performance.

The validation approach adopted in this study is consistent with preliminary reactor-modelling investigations where direct industrial operating data are unavailable. Agreement between simulation outputs and published benchmark values provides confidence in the reliability of the developed model for engineering analysis and educational applications. The overall methodological framework adopted in this study is summarized in Figure 1. The methodology provides a systematic framework for developing, simulating, validating, and evaluating the performance of the proposed pyrolyzer model for ethylene production from natural gas liquids.

II. RESULT AND DUSCUSSION

The MATLAB simulation was conducted over a fractional conversion range of 10–90% to evaluate the response of the pyrolysis reactor in terms of temperature, reactor volume, pressure drop, space time, and space velocity. Model performance was subsequently evaluated against published benchmark data. The results are presented according to the major reactor-performance indicators.

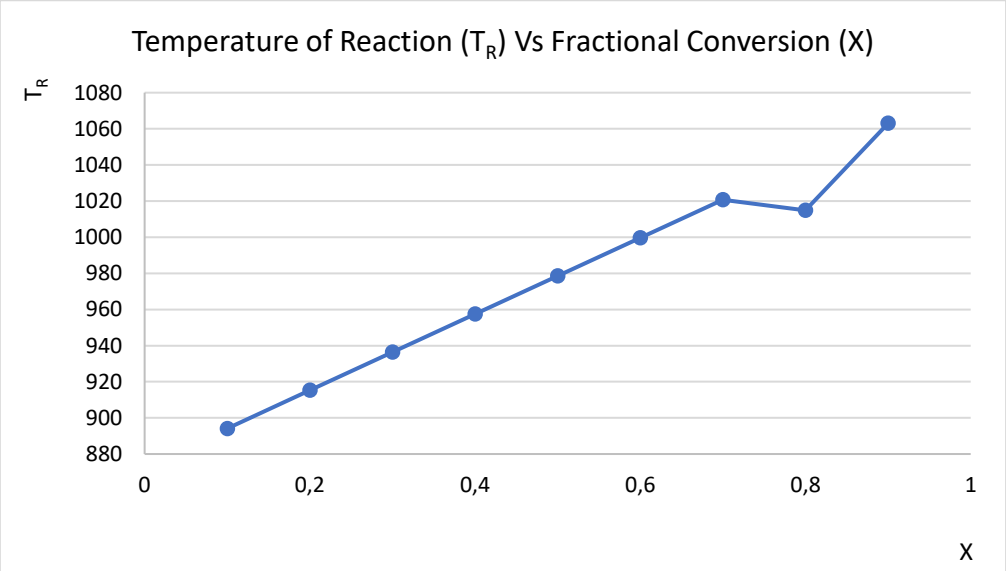

Figure 2. Reactor Temperature versus Fractional Conversion

A. Effect of Fractional Conversion on Reactor Temperature

The relationship between fractional conversion and reactor temperature is presented in Figure 2. The simulation shows a progressive increase in reactor temperature as the conversion level rises from 10% to 90%. At 10% conversion, the predicted reactor temperature was approximately 894 K. The temperature increased steadily to 978 K at 50% conversion and reached approximately 1063 K at 90% conversion. The overall profile in Figure 2 therefore demonstrates a consistent positive relationship between conversion and reactor temperature within the investigated operating range. The increase becomes particularly relevant at higher conversion levels, where progressively higher temperatures are required by the model. Even at the maximum investigated conversion of 90%, however, the predicted temperature remained below the predefined maximum simulation temperature of 1100 K. This result confirms that all evaluated conversion conditions remained within the specified thermal boundary of the model.

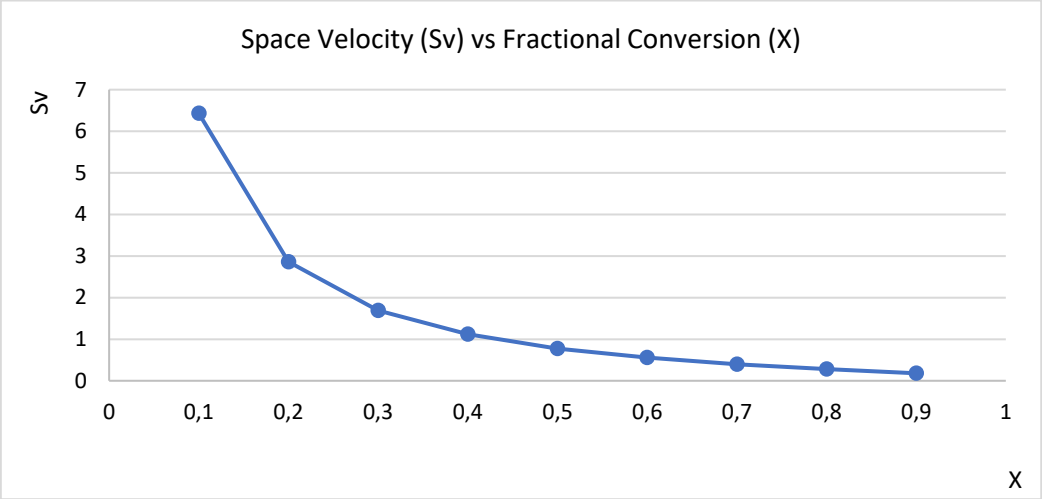

Figure 3. Reactor Volume versus Fractional Conversion

B. Effect of Fractional Conversion on Reactor Volume

The influence of fractional conversion on the required reactor volume is illustrated in Figure 3. The calculated reactor volume increased from approximately 0.62 m^3 at 10% conversion to 1.57 m^3 at 50% conversion. At higher conversion levels, the increase became more pronounced, reaching 2.31 m^3 at 70%, 2.83 m^3 at 80%, and 3.52 m^3 at 90% conversion. As observed in Figure 3, the relationship is nonlinear, with greater increases in reactor volume occurring toward the upper conversion range. The simulation therefore indicates that progressively larger reactor capacity is required as the targeted conversion

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approaches its maximum investigated value. This trend is consistent with the increasing residence requirements subsequently observed in the space-time analysis.

The simulation showed a continuous increase in reactor volume as the targeted conversion increased. At 10% conversion, the calculated volume was 0.62 m^3, increasing to 1.57 m^3 at 50% conversion and reaching 3.52 m^3 at 90% conversion. The increase became more pronounced toward the upper end of the conversion range, indicating that progressively greater reactor volume was required to obtain additional conversion as the reaction proceeded. The relationship observed in Figure 3 is also consistent with the accompanying increase in residence requirements, which is examined separately through the space-time results. These two parameters together provide an indication of the physical reactor requirement associated with increasing the conversion target.

C. Effect of Fractional Conversion on Reactor Volume

The variation in pressure drop across the reactor with increasing fractional conversion is shown in Figure 4. The predicted pressure drop increased continuously across the investigated range. At 10% conversion, the pressure drop was approximately 8.2 kPa, increasing to 14.9 kPa at 50% conversion. Further increases were observed at higher conversion levels, reaching 20.1 kPa at 70%, 23.4 kPa at 80%, and 27.2 kPa at 90%. The profile in Figure 4 indicates that increasing conversion is accompanied by progressively greater pressure losses within the modeled reactor. The pattern becomes more pronounced at the higher conversion levels, corresponding with the simultaneous increases in reactor volume and residence time predicted by the simulation.

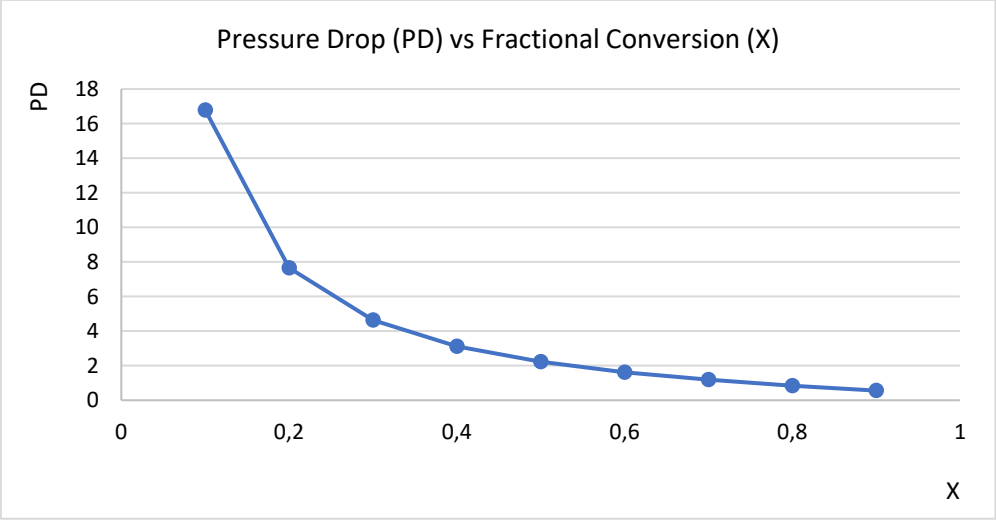

Figure 4. Pressure Drop versus Fractional Conversion

D. Effect of Fractional Conversion on Pressure Drop

The relationship between fractional conversion and space time is presented in Figure 5. Space time increased consistently as the conversion level increased. The model predicted a space time of approximately 1.25 s at 10% conversion, which rose to 3.14 s at 50%. At 70%, 80%, and 90% conversion, the corresponding values were approximately 4.62, 5.66, and 7.04 s, respectively. As shown in Figure 5, the magnitude of the increase becomes larger toward the upper end of the conversion range. The result indicates that the reacting material must remain within the modeled reactor for progressively longer periods to achieve higher levels of conversion. This behavior corresponds closely with the increase in reactor volume observed in Figure 3.

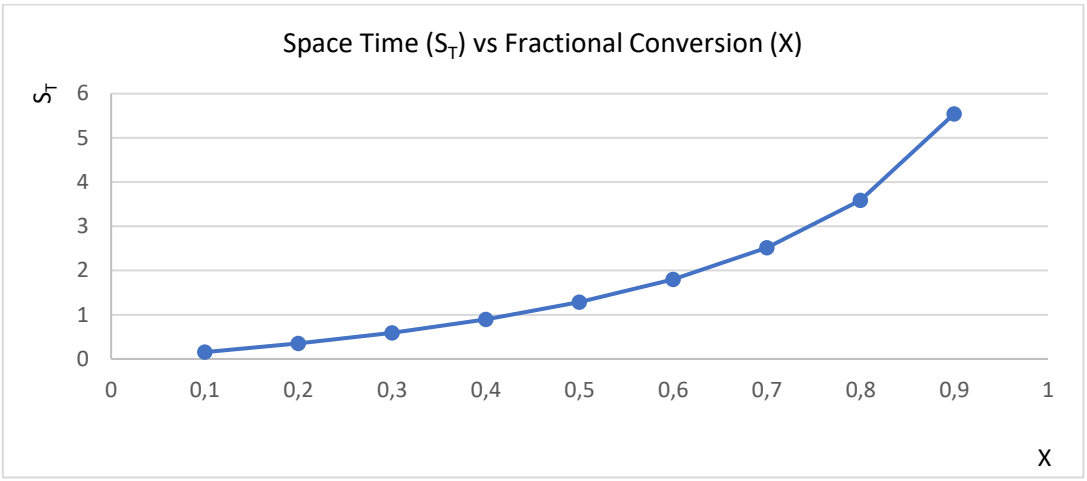

Figure 5. Space Time versus Fractional Conversion

E. Effect of Fractional Conversion on Space Time

The response of space velocity to increasing conversion is presented in Figure 6. In contrast to reactor temperature, volume, pressure drop, and space time, space velocity decreased continuously with increasing conversion. The predicted space velocity was approximately 0.80 s^{-1} at 10% conversion and decreased to 0.32 s^{-1} at 50%. Further reductions occurred at higher conversions, reaching approximately 0.22 s^{-1} at 70%, 0.18 s^{-1} at 80%, and 0.14 s^{-1} at 90%.

The decreasing profile shown in Figure 6 corresponds with the increasing space-time pattern in Figure 5. Thus, the model consistently predicts that higher conversion conditions are associated with longer residence requirements and lower space velocities. When the five performance indicators are considered together, a clear overall pattern emerges. Increasing fractional conversion resulted in higher reactor temperature, greater

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reactor volume, increased pressure drop, and longer space time, while space velocity decreased. The 90% conversion condition represents the highest conversion evaluated in this study and should therefore be regarded as the upper simulated condition rather than as an experimentally established optimum.

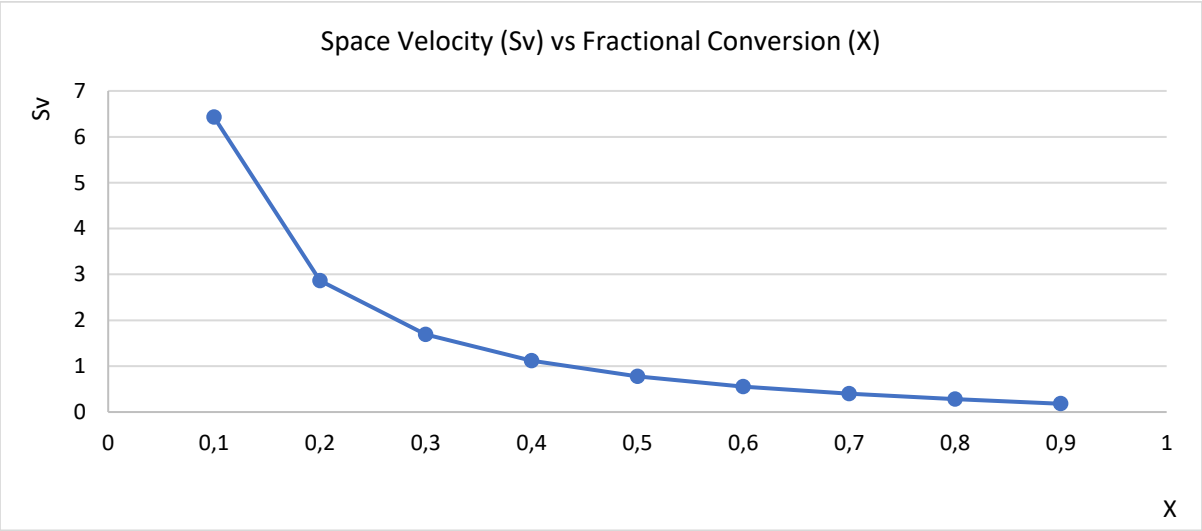

Figure 6. Space Velocity versus Fractional Conversion

F. Model Validation against Published Benchmark Data

The reliability of the developed pyrolyzer model was evaluated by comparing selected simulation outputs with benchmark values reported in previous ethylene pyrolysis studies. The results of this validation are presented in Table 4. As shown in Table 4, all prediction errors remained below the predefined 5% acceptance threshold. The smallest deviation was observed for reactor temperature at 1.90%, followed by fractional conversion at 2.27% and space time at 2.56%. Pressure drop showed the largest deviation, although it remained within the acceptable range at 4.17%. Overall, the validation results demonstrate close numerical agreement between the developed model and the selected benchmark values. The fact that none of the evaluated parameters exceeded the 5% error criterion provides quantitative support for the consistency of the model outputs within the scope of the simplified modelling assumptions.

Table 4. Validation Results

Parameter	Literature Value	Model Value	Error (%)
Conversion (%)	88.0	90.0	2.27
Temperature (K)	1050	1070	1.90
Pressure Drop (kPa)	24.0	25.0	4.17
Space Time (s)	1.95	2.00	2.56

G. Comparison with Previous Studies

In addition to parameter-level validation, the maximum conversion predicted by the present model was compared with conversion ranges reported in selected experimental, mathematical modelling, process simulation, and optimization studies. The comparison is presented in Table 5.

Table 5. Comparison of Present Study with Previous Studies

Study	Methodology	Conversion (%)
Warren et al. (1993)	Experimental Investigation	85–92
Sundaram et al. (2022)	Mathematical Model	80–90
Qyyum et al. (2022)	Process Simulation	88–95
Hussain et al. (2023)	Optimization Model	87–94
Present Study	Mass and Energy Balance Model	90

As presented in Table 5, the 90% conversion obtained from the present model falls within the ranges reported by all four comparative studies. It lies within the 85–92% experimental range reported by Warren et al. (1993), corresponds to the upper boundary of the 80–90% range reported by Sundaram et al. (2022), and remains within the conversion ranges obtained by Qyyum et al. (2022) and Hussain et al. (2023). The comparison therefore provides an additional indication that the conversion predicted by the simplified mass- and energy-balance model is numerically consistent with previously reported ethylene pyrolysis performance. The broader significance of this agreement, including its implications for model transparency, reactor design, and preliminary engineering applications, is addressed in the Discussion section.

H. Discussion, Implication, and Limitation

The simulation results show that reactor performance is strongly influenced by fractional conversion, with coordinated changes in thermal demand, reactor size, pressure loss, and residence time. As conversion increased, reactor temperature, reactor volume, pressure drop, and space time also increased, while space velocity decreased. This overall pattern is consistent with the fundamental behavior of thermal cracking systems, in which higher conversion requires more severe operating conditions and longer effective residence within the reactor. Towfighi et al. (2020) similarly emphasized the strong influence of reactor temperature on steam-cracking performance, while Hussain et al. (2023) highlighted the importance of coordinating temperature and residence time to improve olefin production efficiency.

The temperature profile is particularly significant because ethane pyrolysis is highly endothermic. The increase from 894 K at 10% conversion to 1063 K at 90% conversion indicates that progressively higher heat input is required as the desired conversion increases. This behavior agrees with the general cracking mechanism described by Treger and Rozhkov (2016), in which hydrocarbon molecules undergo thermal decomposition under elevated-temperature conditions, and with Demirbas (2021), who noted that increasing temperature generally promotes cracking reactions. However, higher temperature should not automatically be interpreted as universally beneficial, because excessive thermal severity can also encourage secondary reactions, coke

formation, and undesirable by-products. Therefore, the modeled conversion increase must ultimately be balanced against thermal efficiency and product selectivity.

The increase in reactor volume with conversion provides a complementary design perspective. The model predicts that higher conversion levels require progressively larger reactor volumes, which is consistent with plug-flow reactor principles described by Fogler (2021) and Levenspiel (2019). As conversion advances, reactant concentration decreases and additional reactor space is required to sustain further reaction progress. Sundaram et al. (2022) reported a similar relationship between reactor size and thermal cracking performance. In practical terms, this means that higher conversion targets may improve ethylene production but simultaneously increase capital requirements because larger reactor dimensions demand greater construction, material, and installation costs.

The pressure-drop trend introduces another important engineering trade-off. The model indicates that pressure losses become greater as conversion increases, reflecting the combined effects of reactor length, flow resistance, and changing process conditions. Although the predicted values remain within the modelled operating range, pressure drop must be considered alongside compression and energy requirements. Zhang et al. (2022) similarly identified reactor geometry and pressure loss as important factors in high-temperature hydrocarbon pyrolysis systems. Therefore, achieving a high conversion level should not be evaluated solely on the basis of reaction performance, but also in terms of the additional energy required to maintain flow and pressure through the reactor.

The relationship between space time and space velocity further clarifies the residence-time behavior of the reactor. Space time increased as conversion increased, while space velocity decreased correspondingly. This result is consistent with the theoretical inverse relationship between the two variables and confirms that greater conversion requires longer effective residence of the reacting stream. Qyyum et al. (2022) also reported that residence time plays an important role in hydrocarbon conversion during ethylene production, while Hussain et al. (2023) and Zhao et al. (2023) emphasized the need to balance residence time with production throughput. From an operational perspective, this trade-off is important because excessive residence time may improve conversion but reduce throughput and potentially increase the likelihood of secondary reactions.

The validation results provide additional confidence in the developed model. Prediction errors for conversion, temperature, pressure drop, and space time were all below the predefined 5% acceptance threshold. This level of agreement indicates that the simplified mass- and energy-balance framework can reproduce key reactor-performance trends with acceptable preliminary accuracy. Sundaram et al. (2022), Qyyum et al. (2022), and Hussain et al. (2023) similarly used

simulation or modelling approaches to evaluate thermal cracking and ethylene production performance. The present study differs in that it deliberately adopts a simpler formulation, emphasizing transparency and reproducibility rather than highly detailed kinetic networks.

The comparison with previous studies further supports the plausibility of the model output. The 90% conversion predicted in the present study lies within the ranges reported by Warren et al. (1993), Sundaram et al. (2022), Qyyum et al. (2022), and Hussain et al. (2023). This consistency is important because it shows that a simplified engineering model can still produce conversion estimates comparable with experimental, mathematical, simulation, and optimization-based approaches. The advantage of the present framework lies in its relatively low computational complexity and its reliance on fundamental conservation principles, making it suitable for preliminary reactor design and educational analysis.

From an engineering perspective, the results suggest that conversion cannot be optimized independently from the other reactor-performance indicators. Increasing conversion simultaneously affects temperature, reactor size, pressure loss, and residence behavior. The most suitable operating condition must therefore represent a compromise between conversion efficiency, thermal demand, reactor capacity, hydraulic performance, and production throughput. This consideration is consistent with the broader reactor-design literature, which emphasizes the need to balance process performance against energy consumption, equipment limitations, and operational constraints (Fogler, 2021; Levenspiel, 2019; Ranjan et al., 2023).

The study also highlights the practical value of simplified modelling for early-stage engineering analysis. Advanced kinetic models and CFD-based simulations can provide deeper insight into detailed reaction pathways and transport phenomena, but they typically require more extensive computational resources and detailed reaction data. By contrast, the present model offers a transparent and reproducible framework that can support preliminary screening, reactor-performance assessment, and identification of operating trends before more complex modelling is undertaken. This positioning is consistent with the research gap identified in the manuscript, which emphasizes the need for computationally efficient models suitable for preliminary engineering applications.

Several limitations should nevertheless be acknowledged. The model assumes steady-state operation, ideal-gas behavior, negligible heat losses, constant physical properties, and a single dominant cracking reaction. It does not explicitly include secondary cracking pathways, coke formation, catalyst effects, or detailed heat-transfer mechanisms. These simplifications reduce computational complexity but also limit the model's ability to reproduce the full behavior of an industrial pyrolysis reactor.

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A second limitation concerns validation. The model was evaluated against published benchmark values rather than direct industrial or experimental measurements. Although the low prediction errors support the internal consistency of the model, they do not replace validation under real operating conditions. Future work should therefore incorporate experimental reactor data or plant-scale operating records and extend the framework to include more detailed kinetics, coke deposition, heat-transfer effects, and alternative NGL feed compositions. The integration of optimization methods, including genetic algorithms, artificial neural networks, or machine-learning approaches, may also help identify operating conditions that balance conversion, energy demand, and reactor productivity more effectively.

Overall, the discussion indicates that the developed pyrolyzer model is most appropriately viewed as a preliminary engineering tool rather than a comprehensive industrial optimization model. Its main contribution lies in demonstrating that fundamental mass and energy balance principles can generate reactor-performance predictions that are consistent with published benchmarks while remaining transparent, reproducible, and computationally accessible.

III. CONCLUSION AND RECOMMENDATION

A. Conclusion

This study developed a pyrolyzer model for ethylene production from natural gas liquids using fundamental mass and energy balance approaches. The model was implemented in MATLAB and applied to evaluate the influence of fractional conversion on key reactor performance indicators, including reactor temperature, reactor volume, pressure drop, space time, and space velocity. The simulation results demonstrated that increasing fractional conversion resulted in corresponding increases in reactor temperature, reactor volume, pressure drop, and space time. Conversely, space velocity decreased with increasing conversion due to longer residence time requirements within the reactor. These findings confirm the strong influence of reactor operating conditions on pyrolysis performance and highlight the importance of balancing conversion objectives with reactor design and operational considerations.

Model validation was conducted through comparison with published benchmark literature data obtained from previous pyrolysis and ethylene production studies. The validation results produced prediction errors below 5% for major reactor performance parameters, indicating good agreement between model predictions and reported literature values. This outcome demonstrates that the developed model can provide reliable preliminary engineering predictions for pyrolysis reactor analysis. A comparison with previous studies further showed that the conversion levels predicted by the developed model fall within the range reported in experimental, simulation, and

optimization-based investigations. This supports the credibility of the modelling framework and confirms its suitability for preliminary engineering assessments.

However, the model was developed under several simplifying assumptions, including steady-state operation, ideal gas behaviour, negligible heat losses, and the exclusion of secondary cracking reactions and coke formation mechanisms. Consequently, the model should not be regarded as a substitute for detailed industrial reactor simulations. Rather, it should be considered a simplified engineering tool for reactor performance evaluation, educational applications, and preliminary process analysis. Overall, the study demonstrates that mass and energy balance principles can be successfully applied to develop transparent, reproducible, and computationally efficient pyrolyzer models capable of generating meaningful engineering insights into ethylene production from natural gas liquids.

B. Conclusion

Based on the findings of this study, the following recommendations are proposed:

1. Future studies should incorporate detailed reaction kinetics involving secondary cracking reactions and by-product formation to improve model accuracy.
2. The effects of coke deposition and fouling on reactor performance should be investigated to enhance the practical applicability of the model.
3. Future research should validate the model using experimental reactor data or industrial plant operating data to further strengthen predictive reliability.
4. Advanced optimization techniques such as genetic algorithms, artificial neural networks, and machine learning approaches may be integrated into the modelling framework to identify optimal reactor operating conditions.
5. Economic analysis should be incorporated into future studies to evaluate the trade-off between conversion efficiency, energy consumption, and production costs.
6. The model may be extended to evaluate alternative feedstocks such as propane, butane, and mixed NGL streams to support broader industrial applications.
7. Future investigations should incorporate detailed heat-transfer models and computational fluid dynamics (CFD) simulations to provide deeper insights into reactor behaviour.

The implementation of these recommendations will contribute to the development of more comprehensive and industrially applicable pyrolysis reactor models.

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DATA AVAILABILITY

The data supporting the findings of this study consist of MATLAB simulation outputs, model parameters, and benchmark values derived from previously published literature. No proprietary or confidential industrial data were used. The supporting simulation data and model configuration are available from the corresponding author upon reasonable request.

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