

Article

Neural-Network-Assisted FCC Kinetic Modeling for Enhanced Parameter Estimation Using the CREC Riser Simulator

Jansen Gabriel Acosta-López , Nicolas Torres Brauer  and Hugo de Lasa * 

Chemical Reactor Engineering Centre, Department of Chemical and Biochemical Engineering, The University of Western Ontario, London, ON N6A 3K7, Canada; jacostal@uwo.ca (J.G.A.-L.); ntorres5@uwo.ca (N.T.B.)

* Correspondence: hdelasa@uwo.ca; Tel.: +1-5196612144

Abstract

This study presents an integrated framework for developing kinetic models of vacuum gas oil (VGO) catalytic cracking under sparse experimental data conditions. Experiments were performed in the CREC Riser Simulator at different C/O (catalyst/VGO) weight ratios. The CREC Riser Simulator is a bench-scale mini-fluidized reactor capable of reproducing the short contact times and operating conditions of industrial fluid catalytic cracking (FCC) risers. Product distributions were characterized by using a five-lump scheme consisting of unconverted VGO, light cycle oil (LCO), gasoline, light gases, and coke. To address the limitations associated with sparse datasets, a feedforward neural network (FNN) was used to reconstruct continuous reaction trajectories from discrete experimental measurements. These synthetic trajectories enabled the estimation of kinetic parameters for a phenomenological five-lump reaction network that incorporates catalyst deactivation. The resulting kinetic model established was subsequently implemented in a 1D heterogeneous model of a large-scale industrial FCC riser, providing reliable predictions of VGO conversion, product selectivity, and axial temperature profiles.

Keywords: fluidized catalytic cracking; fluidizable catalysts; CREC riser simulator; kinetic modeling; machine learning

1. Introduction

Nowadays, the development of robust kinetic models is considered a cornerstone of catalytic reaction engineering [1], providing the essential mathematical framework for reactor design, process optimization, and scale-up [2]. However, deriving phenomenologically consistent parameters is a difficult task and remains a major challenge, often hindered by the scarcity and inherent noise of experimental datasets. This is complicated further by the significant number of VGO catalytic cracking reactions that occur simultaneously, among the large numbers of chemical species [3–6].

Traditional regression methods frequently struggle with these limitations, leading to ill-posed inverse problems where the optimizer fails to converge to a global minimum or yields parameters with wide confidence intervals [7–9]. The availability of these phenomenological-based kinetics is also of major importance if one considers the need to evaluate new performing catalysts in the context of promising reactor designs as is the case of catalytic downflow reactors [10,11].

All these topics are particularly significant in the study of complex reaction network schemes [2,5], such as those of the catalytic cracking of vacuum gas oil (VGO). In such fast-reacting systems, the influence of reaction temperature, species partial pressures,



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reaction times, catalyst/oil ratio, and feedstock type on VGO conversion and product selectivity (light gases, gasoline, cycle oil, coke) needs to be determined, using experimental datasets to establish the applicable kinetics [12,13]. It is in this respect that the CREC Riser Simulator [14,15] is a unique and innovative mini-fluidized lab-scale reactor that can be used to evaluate potential new catalysts, given that it reproduces closely the operating conditions of industrial-scale fast fluidized bed riser units.

It is our view that refineries could use the CREC Riser Simulator in their facilities to optimize the performance of their FCC units with the VGOs available and with those to be processed in the foreseeable future (e.g., next few days). In this manner, one can anticipate the suitable kinetics for FCC riser units prior to the VGO refinery processing. However, given the dataset sizes that can be acquired with the CREC Riser Simulator in the short time frame of 2–3 days, it becomes valuable when the datasets obtained are integrated with Machine Learning (ML) [16]. In this respect, Artificial Neural Networks (ANNs) have demonstrated strong capabilities in capturing the non-linear relationships in chemical process data [17,18]. This promising ANN strategy will not be used to replace physical models, but rather to enhance them. By employing ANNs as advanced non-linear interpolators, it is possible to reconstruct continuous reaction trajectories by using sparse experimental points. This “data densification” generates synthetic intermediate values that guide the subsequent parameter estimation, facilitating a more stable data fitting of the mechanistic model.

It is, in this respect, crucial to distinguish this sequential data-augmentation approach from Physics-Informed Neural Networks (PINNs). While PINNs embed the governing differential equations (ODEs) directly into the network’s loss function to constrain the training [19], several studies have reported important limitations associated with this approach, including ill-conditioned optimization problems, sensitivity to loss-weighting strategies, and difficulties in representing multi-scale physical phenomena [20–22]. To circumvent these challenges, the present study adopts a decoupled strategy in which neural networks are used exclusively as non-linear interpolators to densify sparse experimental datasets prior to the regression of a phenomenological kinetic model. This approach preserves the rigorous structure of the mechanistic model while avoiding the convergence difficulties commonly associated with hybrid physics–machine learning loss functions.

In view of the above, the purpose of the present work is to propose a systematic framework for the kinetic modeling of vacuum gas oil (VGO) catalytic cracking, specifically addressing the challenges of parameter estimation under sparse data conditions. Furthermore, by leveraging the Neural Networks, it is proposed to generate high-fidelity intermediate data points from the CREC Riser Simulator experiments, decoupling, in this manner, the data reconstruction process from the mechanistic fitting. Ultimately, the reported methodology demonstrates that a “densified” dataset significantly improves the convergence stability and physical consistency of the kinetic parameters, making it suitable for industrial-scale FCC riser simulation.

To demonstrate the value of this methodology, in this study, the proposed CREC Riser Simulator-Machine Learning derived kinetics is integrated with 1D heterogeneous simulations of an industrial scale riser unit. Thus, the proposed approach shows that only a few simulation minutes are needed to determine the expected VGO conversions, product selectivities, and axial temperature profiles for a selected VGO-FCC catalyst employed in an industrial-scale FCC riser unit in the context of a refinery operation.

2. Results and Discussion

2.1. Catalytic Cracking Results

A significant observation is that there is an upward trend in average VGO conversion and gasoline yield, with increasing C/O ratios (Figure 1), across all experimental runs for the C/O ratios considered in this work (2, 3, 5, and 7). This increase suggests that cracking efficiency is enhanced due to a higher availability of active catalyst sites. These average values provide a consolidated view of product distribution behavior and serve as the basis for the kinetic modeling presented later, in Section 2.3.

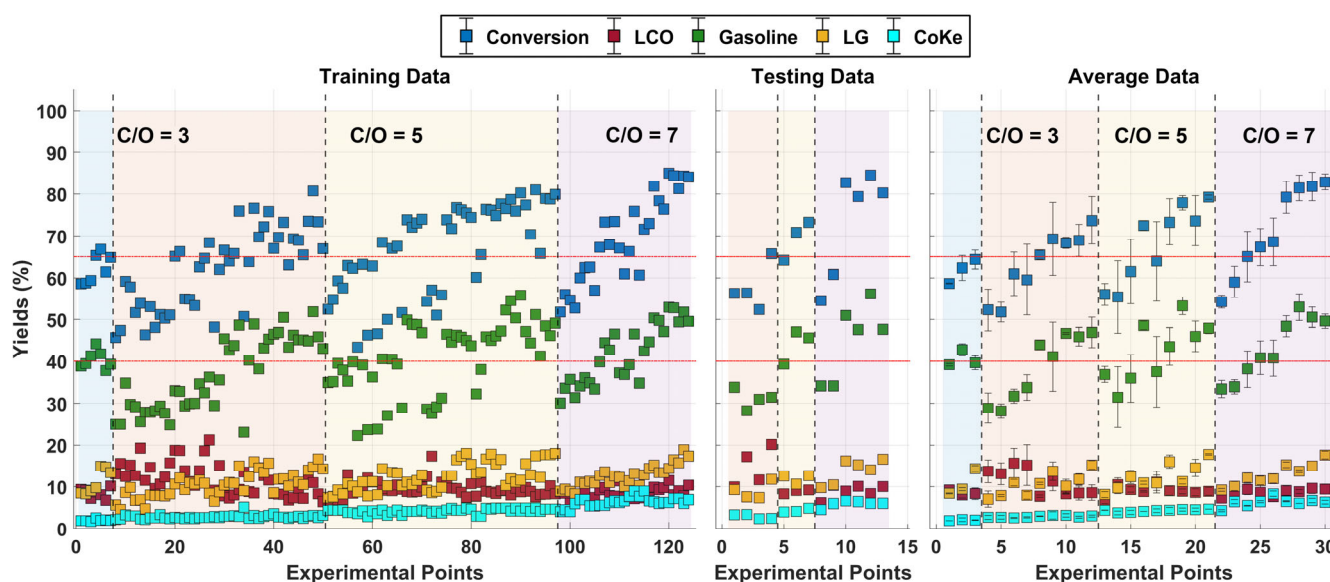


Figure 1. Summary of VGO conversions and product yields across C/O ratio ranges.

Overall, these results illustrate that increasing the C/O ratio leads to a rise in VGO conversion from approximately 40% to over 80%. Meanwhile, gasoline yield also increases, though within a narrower range of 25–45%. Light gases and coke yields grow more moderately, highlighting the trade-off between maximizing conversion and maintaining product selectivity. This trade-off becomes particularly significant between C/O ratios of 5 and 7.

This behavior underscores the importance of carefully optimizing the C/O ratio. As mentioned earlier, although increasing this ratio enhances both VGO conversion and gasoline yield, it simultaneously accelerates secondary cracking reactions and coke formation, which may compromise catalyst stability, cycle oil fraction, and the efficiency of regeneration cycles.

2.2. ANN Model

To evaluate the predictive capability of the model, feedforward neural networks (FNNs) were developed to reproduce the product distributions observed in the experiments. These FNNs were compared against predictions from our previous study [23], while maintaining the same architecture (one hidden layer with 12 nodes and 113 parameters) as a reference. The revised model, however, was trained using a more up-to-date training function, where the influence of the number of iterations on the FCC product lumps was investigated.

As summarized in Table 1, the updated FNN provides a comparable or slightly improved performance on the testing data, with the average R^2 increasing from 0.760 to 0.770 for the higher number of iterations. To prevent overfitting, an intermediate number of iterations was selected for the final model. It is worth mentioning that the resulting

predictions for VGO conversion, LCO selectivity, gasoline selectivity, light gases selectivity, and coke deposition closely match the experimental averages, as illustrated in Figure 2. Overall, the model reproduces the trends observed across all experimental C/O ratios and temperatures, confirming the predictive capability of the FNNs. One can, however, notice the relatively lower R^2 values obtained for LCO that can be attributed to LCO being a relatively minor fraction of the FCC products, making the model performance more sensitive to measurement uncertainty.

Table 1. Product yield predictions by FNN architectures on testing data.

		Previous Study [23] (Acosta-López & de Lasa, 2025)	FNN Low	FNN Med	FNN High
Architecture	Hidden Layers	1		1	
	Nodes	12		12	
	Parameters	113		113	
Main Settings	ANN	feedforwardnet		dlnetwork	
	Train Functions	"traingdx"		dlfeval	
	Iterations	150	150	500	1200
OMSE		0.068	0.086	0.067	0.068
R^2	VGO Conversion (A species)	0.83	0.76	0.81	0.82
	LCO Selectivity (B species)	0.46	0.40	0.50	0.44
	Gasoline Selectivity (C species)	0.77	0.79	0.81	0.79
	Light Gases Selectivity (D species)	0.87	0.85	0.85	0.87
	Coke on Catalyst (E species)	0.87	0.82	0.89	0.90
Average R^2		0.760	0.724	0.772	0.765

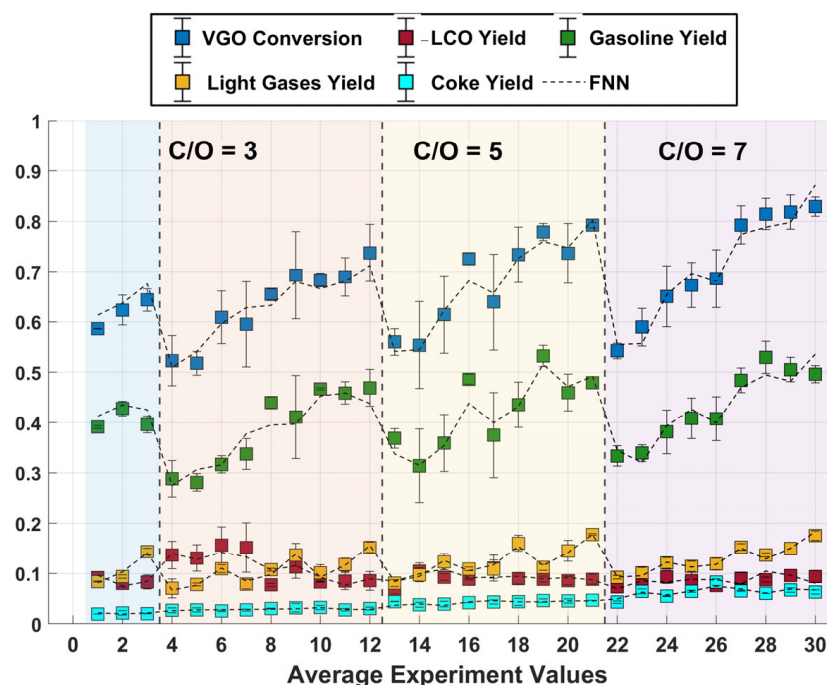


Figure 2. Kinetic model predicted mass fractions (ordinates) versus FNN-experimental mass fractions (abscissas).

The trained FNN was further used to simulate the temporal evolution of mass fractions for each lump species in relation to reaction time, while focusing on C/O ratios ranging from 3 to 7. As shown in Figure 3, the FNN provides a reasonable estimate of the trends

in VGO, LCO, gasoline, light gases, and coke yields over time. The predictions follow the experimental data closely, demonstrating a fast, reliable, and physically consistent representation of product evolution within the shaded zones where experimental measurements were available.

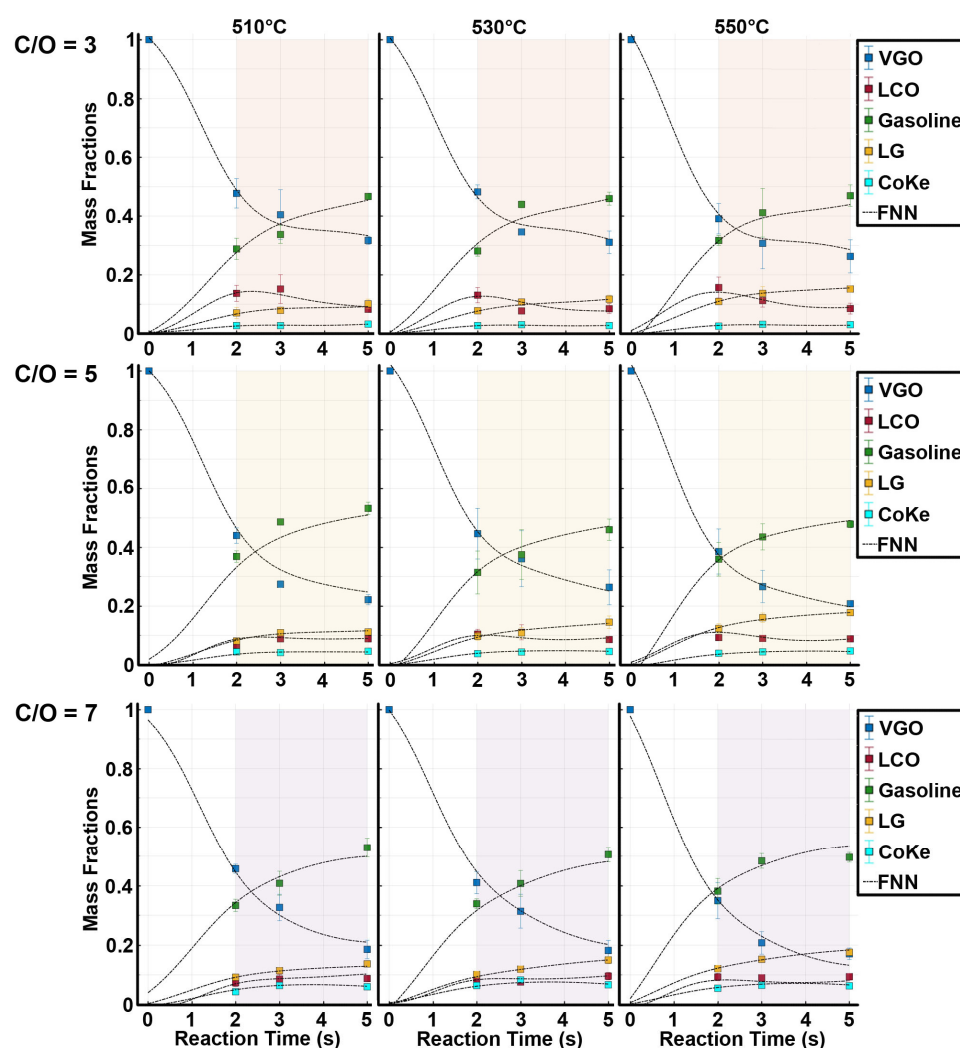


Figure 3. Mass fractions for lump species changes with reaction time. Symbols represent experimental data obtained with the CREC Riser Simulator, and dashed lines indicate the FNN-generated profiles. Note: Shaded zones denote the time intervals where experimental data was acquired, highlighting the agreement between the FNN model and the physical measurements.

Based on the FNN predictions, intermediate points within the shaded zones were set to densify the experimental dataset. This approach increased the number of data points available for subsequent kinetic modeling and non-linear regression, improving the robustness and reliability of the parameter estimation. By leveraging the FNN to guide this data augmentation, the kinetic model could better reproduce the temporal evolution of all lump species across the studied C/O ratios.

Furthermore, these results suggest that integrating data-driven neural networks with experimental measurements can offer a powerful strategy for both understanding and predicting the behavior of the system under study. The FNN can provide rapid and physically consistent estimates of product evolution over time, highlighting its utility as a predictive and decision-support tool in kinetic studies.

2.3. Kinetic Model

A five-lump kinetic model was considered to describe the catalytic cracking of VGO under varying C/O ratios, as described in Section 4.2.1.

2.3.1. Parameter Estimation

The kinetic parameters for the five-lump model were estimated through a robust non-linear regression approach, using experimental data from CREC Riser Simulator runs. The system of model equations was solved using the MATLAB R2026a ODE15s package and the “lsqnonlin” routines, ensuring numerical stability and reliable convergence. In addition, intermediate synthetic points generated from FNN predictions were incorporated to densify the dataset, providing a larger number of reference points for regression. This integration allowed for a more comprehensive comparison between experimental and predicted profiles, enhancing the robustness and reliability of the estimated kinetic parameters. Overall, this modeling approach provides a reliable foundation for analyzing product distribution in FCC processes and serves as a benchmark for the data-driven strategies.

All intrinsic kinetic parameters obtained for the deactivation functions used are reported in Table 2, together with their corresponding 95% confidence intervals (CI). In general, the calculated CI are small. Relative deviations between the estimated parameters and their corresponding CI range from 2% to 30%. This indicates reasonably tight confidence bounds for most of the parameters.

Table 2. Kinetic parameters for VGO catalytic cracking.

	Previous Work [23]		New Kinetic Model (This Study)		Units
	Value	95% CFL	Value	95% CFL	
k_{10}	3.72×10^{-2}	2.54×10^{-3}	3.39×10^{-2}	3.96×10^{-3}	$\text{m}^6/\text{kg}_{\text{Crystallite}}\text{molVGOs}$
E_1	72.24	9.94	76.82	32.66	kJ/mol
k_{20}	2.67×10^{-2}	3.45×10^{-3}	1.74×10^{-2}	4.93×10^{-3}	$\text{m}^6/\text{kg}_{\text{Crystallite}}\text{molVGOs}$
E_2	133.55	9.57	58.14	27.32	kJ/mol
k_{30}	7.27×10^{-3}	7.65×10^{-4}	5.28×10^{-3}	5.95×10^{-4}	$\text{m}^6/\text{kg}_{\text{Crystallite}}\text{molVGOs}$
E_3	70.48	9.44	113.35	40.64	kJ/mol
k_{40}	4.95×10^{-3}	6.66×10^{-5}	8.38×10^{-4}	1.78×10^{-4}	$\text{m}^6/\text{kg}_{\text{Crystallite}}\text{molHCS}$
E_4	100.37	14.78	58.53	31.78	kJ/mol
k_{50}	4.71×10^{-1}	9.37×10^{-2}	3.82×10^{-1}	5.58×10^{-2}	$\text{m}^3/\text{kg}_{\text{Crystallite}}\text{s}$
E_5	33.55	57.31	41.44	36.98	kJ/mol
k_{60}	4.19×10^{-2}	1.25×10^{-2}	3.88×10^{-2}	5.44×10^{-3}	$\text{m}^3/\text{kg}_{\text{Crystallite}}\text{s}$
E_6	146.97	74.17	76.93	42.29	kJ/mol
D_o^*	15.65	0.80	13.67	2.68	m^2/s
E_D	47.52	8.48	52.85	15.52	kJ/mol
λ/X_E	0.05	4.49×10^{-3}	0.08	1.47×10^{-3}	-

* Notes: (a) Values of D_o are multiplied by a 10^{13} factor, (b) $ki = ki0 \exp(Ei(1/T - 1/To))$.

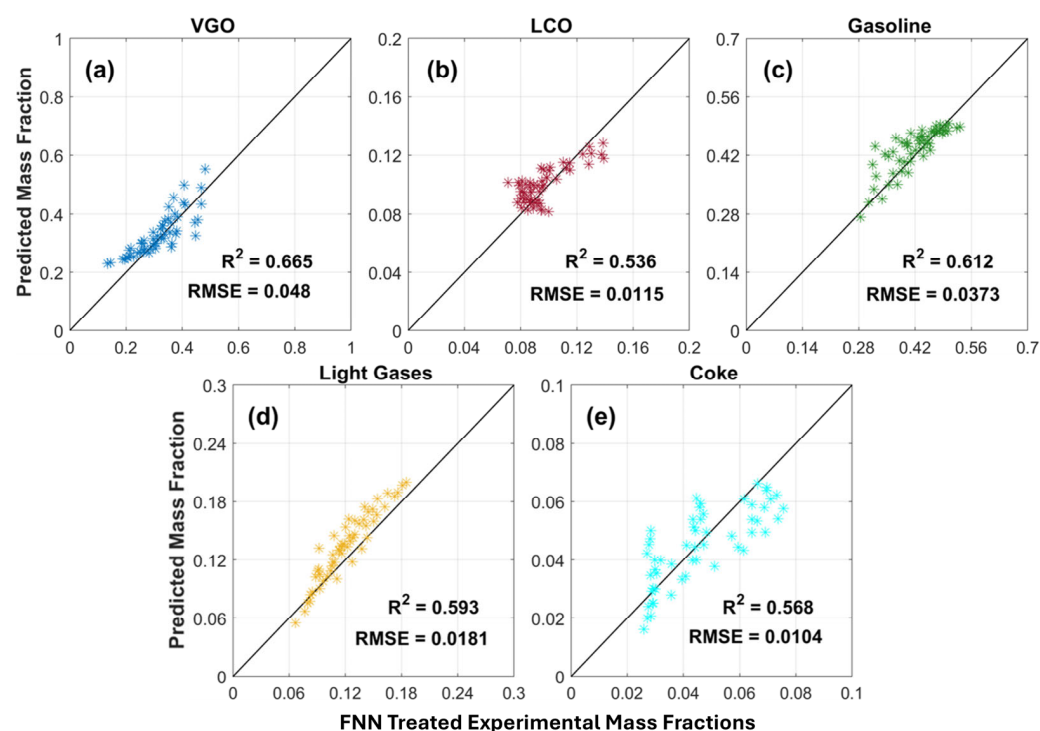
2.3.2. Yields of Products—Kinetic Model Predictions

This section reviews the different kinetic model predictions, as reported in Table 2, on the basis of both lump prediction yields and R^2 regression coefficients.

One can observe in Table 3 and Figure 4 that the average R^2 increases significantly from 0.53 to 0.57 and 0.60. This reflects the fact that the new kinetic model reported here outperforms the previous Jansen and de Lasa model (2025) with respect to the LCO and coke fractions. Moreover, one can also see that there is a recommended number of 63 testing points at various C/O ratios in order to obtain trustable model predictions.

Table 3. Comparison of product lump prediction using two different kinetics, as well as two sizes of data samples.

	Previous Work [23]	New Kinetic Model (This Study). Smaller Data Sample	New Kinetic Model (This Study). Larger Data Sample
C/O Range	2 to 7	3 to 7	3 to 7
Testing Points	27	27	63
MSE	0.068	0.081	0.068
R^2	Converted VGO	0.73	0.67
	LCO	0.15	0.54
	Gasoline	0.62	0.61
	Light Gases	0.83	0.59
	Coke	0.31	0.57
Average R^2	0.527	0.536	0.600

**Figure 4.** Kinetic model predicted mass fractions (ordinates) versus FNN-treated experimental mass fractions (abscissas) for: (a) unconverted VGO (dark blue), (b) LCO (pink), (c) gasoline (green), (d) light gases (gold) and (e) coke (light blue) for new kinetic model + synthetic data.

2.3.3. Industrial Scale Model Predictions

With the kinetic parameters of the proposed VGO cracking reaction adjusted, a simulation of a large-scale FCC riser reaction unit was carried out, as described in Section 4.2.2. To accomplish this, the simultaneous numerical solutions of Equations (A1)–(A5) of Appendix A and Equation (21) were required. The thermal and thermodynamic parameters needed for Equation (21) and Equation (A6) are provided in Appendix B.

Numerical simulation results were affected at 3, 5 and 7 C/O ratios, at a mixing feed temperature of 550 °C. Outcomes of the simulations are reported in Figure 5a for C/O = 3, Figure 5b for C/O = 5 and Figure 5c for C/O = 7.

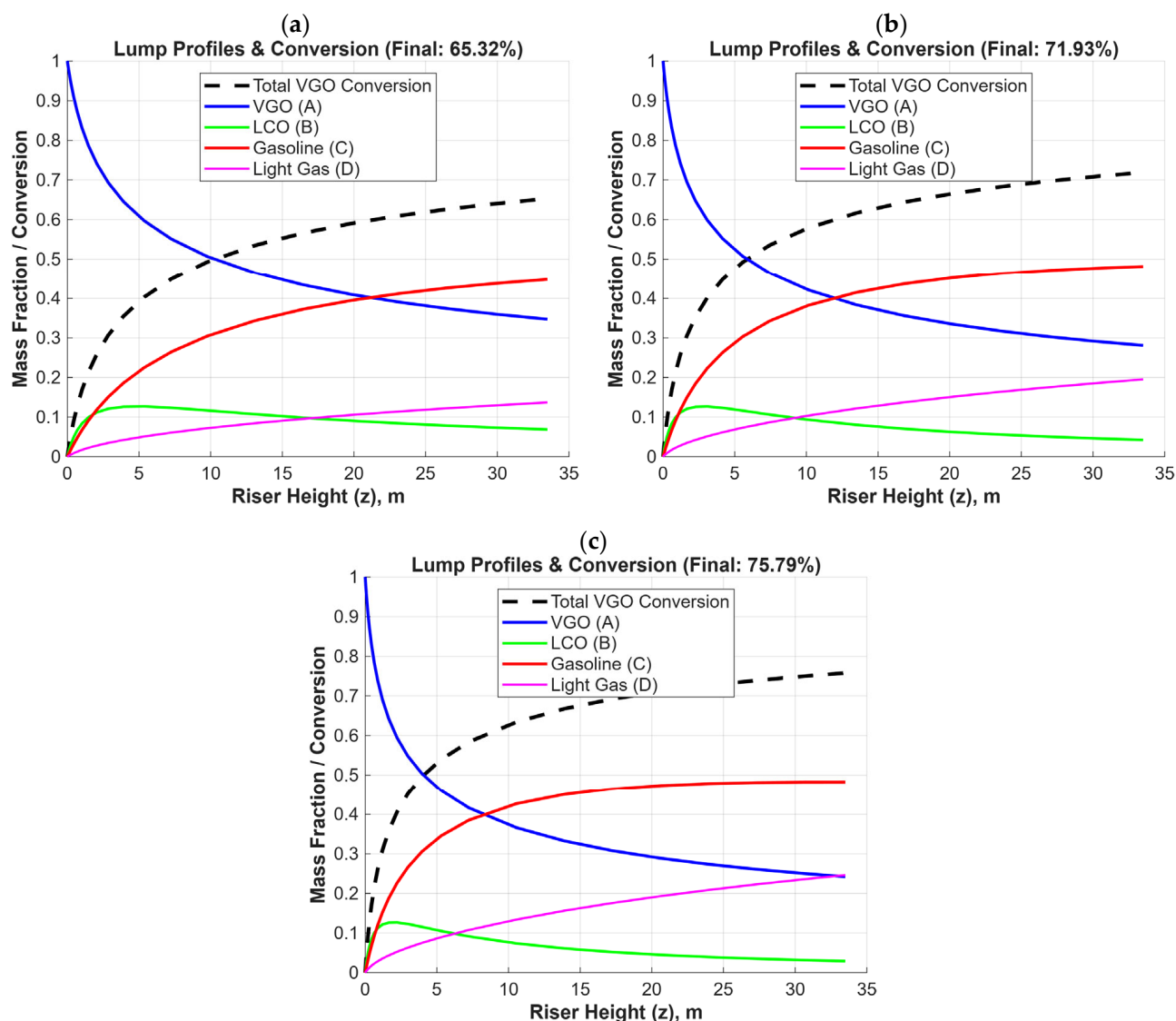


Figure 5. Mass fractions of various catalytic cracking lumps along the length of an industrial riser. Notes: (a) for C/O = 3, (b) for C/O = 5, (c) for C/O = 7, diameter of the reaction zone section: 1.25 m, $F_{VGO} = 29$ Kg/s, mixing temperature at the entry of the riser reaction zone: 550 °C.

Figure 5a–c show that in increasing the C/O ratio, while maintaining a constant inlet mixing temperature of 550 °C, there is a progressive increase in both outlet VGO conversion and coke formation, rising from 65.32% to 76.37% and from 0.94% to 1.33%, respectively. Furthermore, significant changes are observed in the cycle-oil-to-gasoline fraction ratio as the C/O ratio increases, with this ratio decreasing from 15% to 6%, once the C/O is increased from 3 to 7. Another significant change is observed for the light gases with this lump being segmented from 13.7% to 24.6%. In contrast, and for the same change in C/O ratio, gasoline yield remains relatively constant, within the range of 44.7–48.2%. Furthermore, Table 4 reports the overall FCC riser temperature drop together with the coke-on-catalyst for various C/Os.

In summary, these FCC unit scale-up results, based on catalytic cracking kinetics derived from data obtained using the reliable CREC Riser Simulator and kinetic parameters carefully determined through FNN analysis, demonstrate the significant impact of changes in the catalyst-to-oil (C/O) ratio on the performance of an industrial-scale FCC unit. The results indicate that the catalyst-to-oil (C/O) ratio is a critical operating parameter for

optimizing FCC unit performance, particularly in the context of an evolving fuel market and the anticipated increase in diesel fuel demand.

Table 4. Temperature axial change in the riser and coke yield at the riser outlet at C/O ratios of 3, 5 and 7.

C/O	$T_{mix}(^{\circ}\text{C})$	$T_{Out}(^{\circ}\text{C})$	ΔT_{riser}	Coke Production (kg/s)	w% Coke/Catalyst	% of VGO Feed
3	550	506.3	−43.7	1.140	1.33	3.99
5	550	508.8	−41.2	1.566	1.10	5.48
7	550	511.9	−38.1	1.885	0.943	6.60

3. Experimental Methods

3.1. Procedure and Apparatus

Catalytic cracking experiments were performed in a CREC Riser Simulator (RS) invented at the Chemical Reactor Engineering Centre (CREC-UWO). This laboratory-scale unit, designed by H. I. de Lasa (1992) in London, Ontario, Canada, and enhanced significantly in 2019 [15,24], accurately simulates an industrial FCC riser unit, thus making possible the testing of catalysts and the development of kinetic models for the cracking of heavy oil fractions such as VGO. As shown in Figure 6, the CREC Riser Simulator contains an upper shell and a lower shell, which together allow the catalyst to be easily loaded into and unloaded from a basket in the lower shell of the reactor.

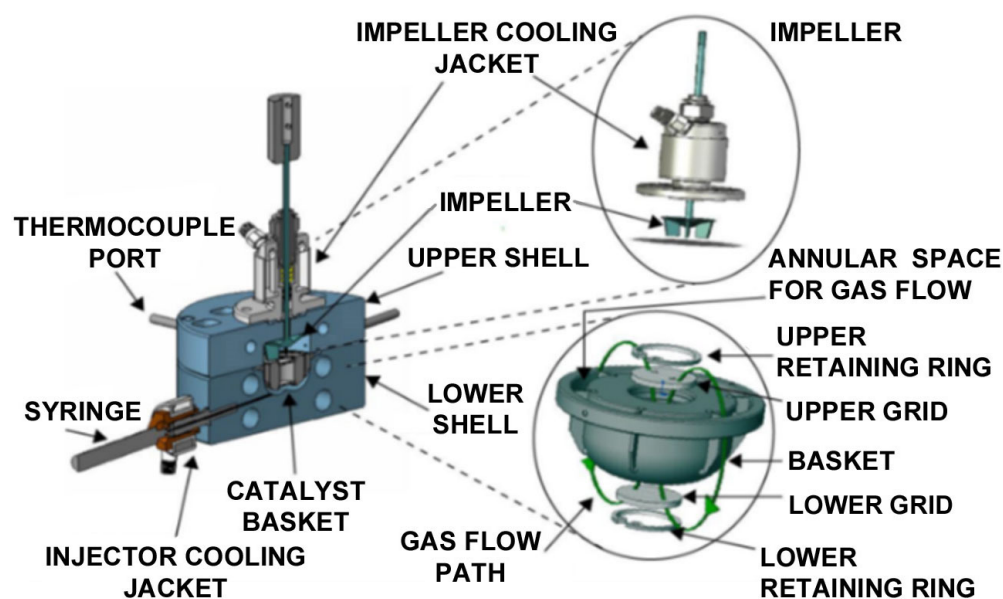


Figure 6. Description of the 1992-CREC Riser Simulator and its various components [25].

The mini-fluidized bed of the CREC Riser Simulator (Figure 6) operates in conjunction with other accessories, such as a vacuum box, a gas chromatograph (GC), a series of sampling valves, a timer, two pressure transducers and two temperature controllers. As described in Figure 7, the auxiliary equipment includes the following: (a) a 4-port valve that enables the connection and isolation of the 54 cm³ reactor to the 1000 cm³ vacuum box; (b) a 6-port valve with a sampling loop that allows samples of reaction products to be collected; (c) a mass flow controller; (d) temperature-controlled heated lines that allow for the adequate transfer of chemical species without condensation; and (e) pressure gauges [25,26]. These components allow the precise control of (a) reaction times (2–7 s),

(b) temperatures (500–575 °C), and (c) catalyst-to-oil or C/O ratios (1–9) at various VGO partial pressures, while enabling the rapid evacuation of reaction products. At the end of the experiment, reaction samples are directed to the GC for FID and TCD analysis, allowing the quantification of hydrocarbons and the determination of carbon balances for each run.

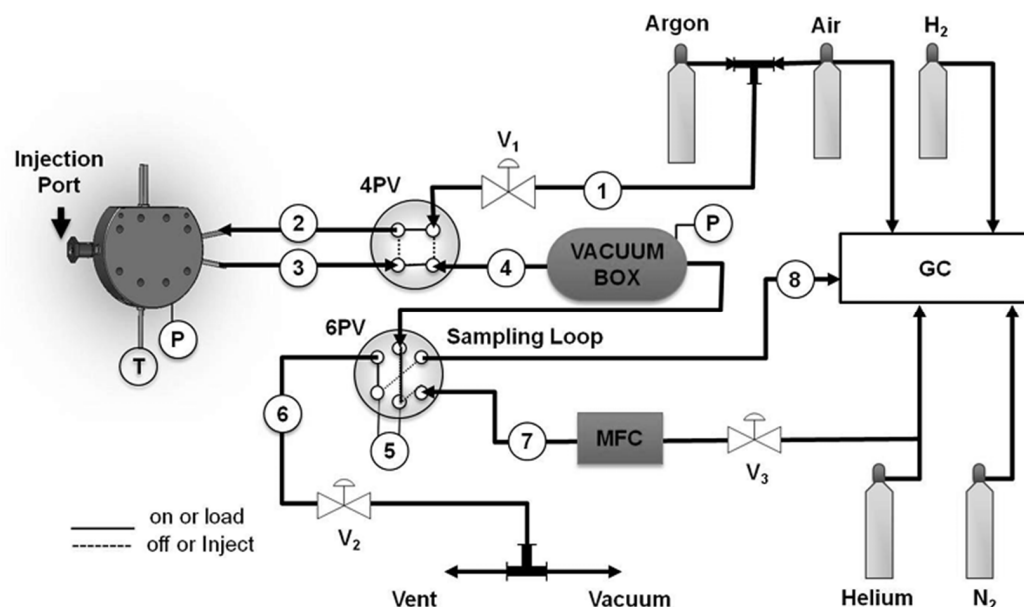


Figure 7. Schematic diagram of the CREC Riser Simulator experimental setup from Alkhlel, 2019 [27].

Catalytic Cracking Experiments

Catalytic cracking runs using VGO were conducted at three temperatures: 510, 530, and 550 °C; three reaction times: 3, 5, and 7 s; and five C/O ratios: 1, 2, 3, 5, and 7. A 5-lump model including the unconverted VGO, the light cycle oil (LCO), the gasoline, the light gases, and the coke was employed to estimate the main product fractions. This 5-lump model was chosen due to its ease of implementation compared to more complex alternatives [12]. The five lumps considered for this study were classified based on boiling point (BP) ranges, as reported in Table 5. The VGO feedstock was obtained from Imperial Oil Limited, located in Sarnia, Ontario, Canada [10].

Table 5. Properties of proposed lump species.

Lump	Boiling Point Range at 1 atm (°C)	Molecular Weight (g/mol)	Range of Hydrocarbons
VGO (A species)	>342.7	340	>C ₂₆
Light cycle oil (B species)	216.3–342.7	226	C ₁₂ –C ₂₆
Gasoline (C species)	36.1–216.3	114	C ₅ –C ₁₂
Light gases (D species)	<36.1	44	C ₁ –C ₄
Coke (E species)	-	12.7 *	CH _{0.7}

* The molecular weight assigned to the coke species is based on the CH_{0.7} coke elemental composition formula.

The experiments were performed using a 0.18 g VGO sample that was injected with the catalyst weight-loading adjusted to achieve the desired C/O ratios. The VGO conversion (X_{VGO}) and product yield (Y_i), were calculated using the following equations:

$$X_{VGO} = \frac{W_{VGO,o} - W_{VGO}}{W_{VGO,o}} \quad (1)$$

$$Y_i = \frac{W_i}{W_{VGO,o} - W_{VGO}} \quad (2)$$

where $W_{VGO,o}$ is the weight of injected VGO; W_{VGO} is the outlet mass of unconverted VGO; and W_i is the estimated mass of each lump i .

Each cracking reaction experimental condition was repeated 2–3 times to ensure that the results were consistent, reproducible and statistically sound. The 54 cm³ constant volume CREC Riser Simulator reactor with a typically 1 g catalyst-loading was operated isothermally at a specified total reaction time (2 s to 5 s). The FCC catalyst used, designated as Catalyst A, was an equilibrium catalyst, with its XRD, N₂-BET, NH₃-TPD, and pyridine adsorption FTIR properties, reported in Alkhlel & de Lasa (2019) [28]. A total of 197 runs, including repeated experiments, were conducted. The experimental results were validated through mass balance calculations by using argon as an internal standard, which ensured the consistency of hydrocarbon product estimations, across the different stages of the CREC Riser Simulator operation. The details of these mass balance calculations, with carbon balances closing at 91.2% with a standard deviation of $\pm 2.4\%$, were described in our previous study [23].

4. Modeling

4.1. AI-Based Modeling

In recent decades, there has been a growing trend toward implementing Artificial Intelligence (AI)-based models for data extraction and analysis in chemical processes [16]. Among these, ML algorithms have gained particular attention for their ability to learn patterns from data and make accurate predictions. As a result, ML techniques have been widely deployed across process industries, especially for process monitoring, control, and optimization [18].

Artificial Neural Network (ANN)

Given their ability to “learn” hidden patterns from input-output process data, ANNs have become one of the most widely used ML algorithms in various industrial applications. Furthermore, due to their high potential for handling non-linear relationships through different activation functions, neural networks have gained considerable interest across the different fields of chemical processes [16,17]. More recently, our research team accomplished progress in the application of ANNs to catalytic cracking [23,29]. The present study represents a further contribution in this respect with a special emphasis being placed on concurrent kinetic modeling and machine approaches for better parameter estimation and large-scale FCC riser simulation.

4.2. Kinetic Modeling

4.2.1. FCC Reaction Network

The kinetic model for VGO catalytic cracking is developed using a five-lump approach that includes VGO (C26–C40), light cycle oil or LCO (C12–C26), gasoline (C5 $\pm$ C12), light gases (C1–C4), and coke. It accounts for the influence of catalyst deactivation and C/O ratio. The proposed five-lump model considers six primary simultaneous reactions that describe the reaction pathways for the VGO, the LCO lump, the gasoline lump, the light gases lump, and the coke lump, as illustrated in Figure 8.

In the revised network, based on the original network from Al-Sabawi et al. (2006) [12] as shown in Figure 8, coke formation is modeled as a second-order condensation reaction involving VGO, LCO, and gasoline. This modification ensures that coke yield changes consistently with C/O ratio, making the resulting set of equations and their kinetic parameters applicable across the entire range of catalytic cracking conditions and suitable for large-scale riser simulations, as reported later in this study.

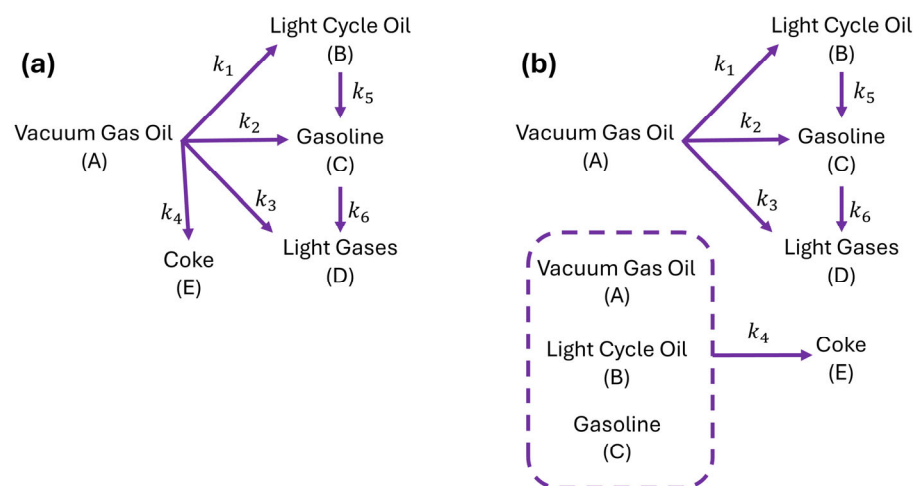


Figure 8. Five-lump catalytic reaction network: (a) original network from Al-Sabawi et al. (2006) [12] and (b) revised network developed in this work.

4.2.2. Kinetic Modeling in CREC Riser Simulator

Catalytic cracking in a mini-fluidized CREC Riser Simulator can be described by using an ideal batch reactor model [30]. This model is suitable, given that it accounts for an intense gas-phase mixing of reactants and products, as well as for the expected catalyst fluidization that occurs in the reactor [25]. Thus, the consumption of VGO in the well-mixed batch reactor can be represented by the species balance shown in Equation (3) [12]. This formulation is supported by the assumption that both adsorption and reaction phenomena occur within the zeolite crystals, while the catalyst matrix remains inert, as proposed by Al-Khattaf et al. (2002) [31].

$$-\frac{V}{W_{cr}} \frac{dC_A}{dt} = \eta_{ss} r_A \quad (3)$$

where r_A is the rate of the consumption of VGO in the absence of diffusion control; η_{ss} is the effectiveness factor; C_A represents the concentration of VGO; W_{cr} is the weight of zeolite crystals; and V is the total reactor volume.

Furthermore, as shown in Equation (4), the rate of VGO consumption, r_A , is normally described using a second order reaction rate [30,32]. This assumption is based on the reactivity of the gas oil molecules, given that at low VGO conversions, the most reactive molecules crack more readily and, as the conversion of VGO increases, the reactivity of the feed molecules decreases [26]. Thus, the following equation can be used to describe the five-lump reaction network pathway for VGO, considering the network of Figure 8b:

$$r_A = \eta_{ss} \varphi (k_1 + k_2 + k_3) C_A^2 \quad (4)$$

where φ is the catalyst activity decay due to coke deposition; and k_1 , k_2 , k_3 , and k_4 are the intrinsic rate constants, considered in the reaction network.

Moreover, the concentration of VGO in the CREC Riser Simulator, represented by C_A , can be related to the mass fraction of VGO in the CREC Riser Simulator at any reaction time. This is described by the following equation:

$$C_A = \frac{y_A W_{VGO}}{MW_A V} \quad (5)$$

where y_A is the mass fraction of VGO; W_{VGO} is the weight of liquid feedstock injected into the reactor; and MW_A is the molecular weight of VGO. Thus, the consumption of VGO

in the CREC Riser Simulator (Equation (6)) can be evaluated in terms of mass fractions, as follows:

$$-\frac{V}{W_{cr}} \frac{dy_A}{dt} = \eta_{ss} \varphi \left(\frac{W_{VGO}}{MW_A V} \right) (k_1 + k_2 + k_3) y_A^2 \quad (6)$$

Additionally, each intrinsic kinetic constant, represented by k_i , can be represented by an Arrhenius-type equation:

$$k_i = k_{i0} \exp \left[\frac{-E_i}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] \quad (7)$$

where k_{i0} is the pre-exponential factor; E_i represents the energy of activation; and T_0 is the 530 °C centering temperature. As mentioned by Usman et al. (2017) [32], incorporating the centering temperature into the conventional Arrhenius equation allows one to reduce the parameter interaction between k_{i0} and E_i . This is particularly convenient when conducting non-linear regression analyses.

Similarly, species balances can be established for the remaining four lumps, with these balances containing formation and/or consumption terms for each lump. In the case of LCO and gasoline, which have narrower boiling ranges than VGO, the cracking rates can be modeled using first-order reactions [12]. Thus, the balance for the LCO lump includes two terms, one for the formation of LCO which is the result of VGO cracking, and the other for the consumption of LCO:

$$\frac{V}{W_{cr}} \frac{dC_B}{dt} = \varphi (\eta_{ss} v_B k_1 C_A^2 - k_5 C_B) \quad (8)$$

$$\frac{V}{W_{cr}} \frac{dy_B}{dt} = \varphi \left[\eta_{ss} v_B \left(\frac{W_{HC}}{MW_A V} \right) \left(\frac{MW_B}{MW_A} \right) k_1 y_A^2 - k_5 y_B \right] \quad (9)$$

The rate equation for gasoline formation contains three terms. Two correspond to the formation of gasoline as result of VGO and LCO lump cracking, and the remaining one corresponds to the consumption of gasoline, due to cracking:

$$\frac{V}{W_{cr}} \frac{dC_C}{dt} = \varphi (\eta_{ss} v_C k_2 C_A^2 + \frac{v_C}{v_B} k_5 C_B - k_6 C_C) \quad (10)$$

$$\frac{V}{W_{cr}} \frac{dy_C}{dt} = \varphi \left[\eta_{ss} v_C \left(\frac{W_{HC}}{MW_A V} \right) \left(\frac{MW_C}{MW_A} \right) k_2 y_A^2 + \frac{v_C}{v_B} \left(\frac{MW_C}{MW_B} \right) k_5 y_B - k_6 y_C \right] \quad (11)$$

Additionally, the following equations are used to describe the formation of light gases and coke:

$$\frac{V}{W_{cr}} \frac{dC_D}{dt} = \varphi (\eta_{ss} v_D k_3 C_A^2 + \frac{v_D}{v_C} k_6 C_C) \quad (12)$$

$$\frac{V}{W_{cr}} \frac{dy_D}{dt} = \varphi \left[\eta_{ss} v_D \left(\frac{W_{HC}}{MW_A V} \right) \left(\frac{MW_D}{MW_A} \right) k_3 y_A^2 + \frac{v_D}{v_C} \left(\frac{MW_D}{MW_C} \right) k_6 y_C \right] \quad (13)$$

$$\frac{dX_E}{dt} = \varphi (\eta_{ss} v_E MW_E k_4 C_T^2) \quad (14)$$

$$\frac{V}{W_{cr}} \frac{dX_E'}{dt} = \varphi \left[\eta_{ss} v_E \left(\frac{W_{HC}}{MW_A V} \right) \left(\frac{MW_E}{MW_A} \right) k_4 y_T^2 \right] \quad (15)$$

where k_T represents the kinetic constant involved in coke formation and C_T stands for the sum of coke precursor concentration species involving A, B and C species.

In the above equations, v_i represents the stoichiometric coefficient for lump i , and X_E is the mass of coke produced, per unit mass of crystallites and X_E' , the mass of coke formed, per unit mass of VGO. Note that $\sum y_i + X_E' = 1$. Furthermore and consistent with Figure 8b,

Equation (6), (8) and (10) neglect the changes in molar fractions of VGO, LCO and gasoline due to coke formation.

Furthermore, it is expected that the diffusion of VGO in the USY zeolites falls under the configurational ('intracrystalline') diffusional regime [33], which corresponds to an activated, temperature-dependent mechanism. As suggested by Al-Khattaf et al. (2002) [31], this mechanism can be described by the Eyring equation, which defines the effective diffusivity (D_{Eff}) as follows:

$$D_{Eff} = D_o \exp \left[\frac{-E_D}{R} \left(\frac{1}{T} - \frac{1}{T_o} \right) \right] \quad (16)$$

As highlighted by Al-Sabawi et al. (2006) [12], under specific conditions such as elevated temperatures, the catalytic cracking of gas oil becomes less sensitive to crystallite size, with diffusional limitations within the zeolite pore structure having minimal impact on the overall reaction rate. In contrast, at lower temperatures, diffusional effects become significantly more pronounced. In this context of the present work, the effectiveness factor (η_{ss}), as defined in Equations (17) and (18), is expected to approach unity at higher temperatures. This is consistent with the anticipated behavior of the Thiele modulus under such conditions.

$$\eta_{ss} = \frac{r_{mean}}{-k_i C_i^n \big|_{r=R_{cr}}} \quad (17)$$

$$\eta_{ss} = \frac{\tanh(h'_i)}{h'_i} \quad (18)$$

In the case of the VGO cracking over USY zeolites after the modified reaction network of this study, the modified Thiele modulus (h'_{VGO}) can be expressed as:

$$h'_{VGO} = \frac{L}{6} \sqrt{\left(\frac{n+1}{2} \right) \frac{\varphi(k_1 + k_2 + k_3) C_A \rho_{cr}}{D_{Eff}}} \quad (19)$$

where L is the characteristic dimension of the zeolite crystallite; ρ_{cr} is the density of the USY zeolite crystallite; and n_r represents the reaction order adopted for the VGO consumption.

Regarding the coke deposition, a non-selective deactivation function (φ) is proposed in this work. In this scenario, catalyst deactivation is related to the catalyst sites covered by coke. This formulation follows a second-order condensation reaction involving VGO, LCO, and gasoline, as expressed by Equation (20):

$$\varphi = 1 - \left(\frac{X'_E}{X_{Ec}} \right)^2 \quad (20)$$

where X'_E represents the mass of coke produced per mass of gas oil injected and X_{Ec} represents the maximum expected (critical) coke yield, estimated at long reaction times, under the experimental conditions considered.

4.3. Industrial Scale Simulation

The primary objective of the FCC riser reactor simulation is to calculate the concentrations of the principal oil species of interest and to evaluate the riser reactor performance. In this work, the FCC riser performance evaluation is based on VGO conversion and on the yields of various hydrocarbon products, which result from primary VGO cracking and from the secondary cracking reactions of gasoline and cycle oil species.

Considering that the extent of the cracking of hydrocarbon species mainly depends on the gas–solid residence time, the amount of available catalyst surface, the partial pressures

of various hydrocarbon species, and the heat transfer from the catalyst [34], one must therefore account for the kinetics, the thermodynamics, and the fluid dynamics of VGO catalytic cracking in order to adequately represent the operating conditions in the FCC riser unit. This is required to accurately calculate the flow properties, including the gaseous species and the catalyst particle concentrations.

Accordingly, simulations were developed for an industrial-scale FCC riser reactor unit, characterized by dimensions of 0.96–1.25 m in diameter with a height of 43 m, and with a 32.5 m reaction zone length below the VGO injectors. These specific unit dimensions were taken from the FCC unit of the Petronor S. A. Refinery, situated in Bilbao, Spain, as reported by Arandes et al. (2000) [35]. Figure 9 provides an overview of the boundary conditions (BC) required for the continuous FCC riser unit simulations.

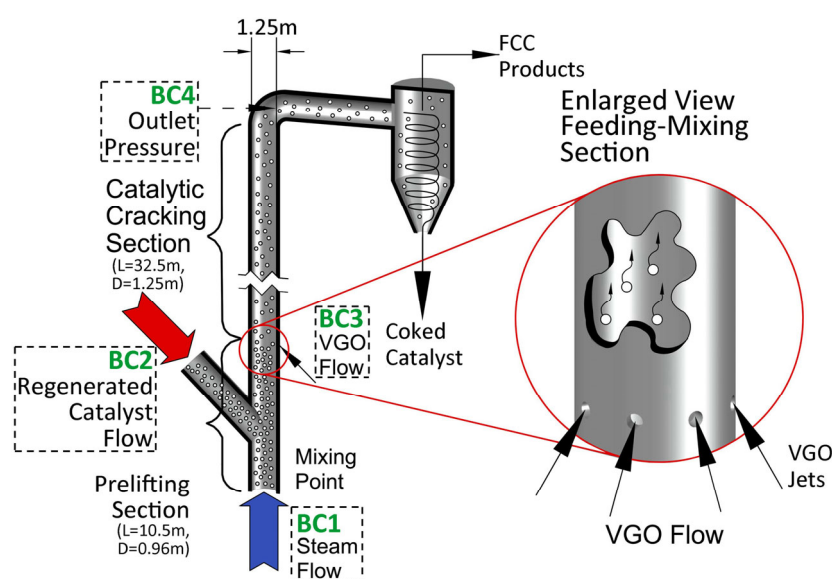


Figure 9. Geometry and boundary conditions of the FCC riser reactor unit. Notes: BC1: Steam incoming flow; BC2: regenerated catalyst flow, BC3: VGO incoming flow, BC4: outlet pressure [29].

FCC Proposed Model 1D Heterogenous Model for the Industrial Scale Unit

In order to proceed with the calculations to simulate an industrial scale unit operation, the present work considers the same equations as listed in Section 4.2.2. A MATLAB-R2026a script is used, while including the differential reaction time as shown in Equations (9), (11), (13) and (15) for the various species, at different incremental axial positions. In order to conform with the non-isothermal operation of the industrial scale riser, another equation is added to the equation set. This equation accounts for the differential thermal balance in the industrial riser unit.

$$\frac{dT}{dz} = - \frac{Q_{cracking}(1 - \epsilon)\gamma\rho_{catalyst}A}{(F_t C_{p,gas} + F_{catalyst} C_{p,catalyst})} \quad (21)$$

with $Q_{cracking}$ being the combined heat of cracking for the various steps of the catalytic cracking, $(1 - \epsilon)$ the volumetric concentration of catalysts, γ the crystallites weight fraction in the FCC catalyst, $\rho_{catalyst}$ the apparent catalyst density, F_t the combined mass flow of steam and hydrocarbons, $F_{catalyst}$ the catalyst mass flow, $C_{p,gas}$ the specific heat capacity for the combined steam and hydrocarbon, and $C_{p,catalyst}$ the specific heat capacity for the catalyst.

To solve these equations which encompass the 1D heterogenous model proposed, several modeling assumptions were made, as follows:

- The fluid flow in the FCC riser unit can be adequately represented by two phases (gas-phase hydrocarbons and catalyst), given the minor influence of feedstock droplet vaporization at the injection zone.
- The adiabatic reactor model is appropriate for establishing the enthalpy balances in the FCC riser unit, considering that heat losses typically remain below 5% in this type of reactor, under well-insulated conditions.
- Thermodynamic properties such as heat of formation and heat capacity of both fluid and catalyst phases were approximated using predefined parameters.
- The gas and catalyst phases are moving in the FCC riser at the same velocities, an approximation which neglects the slip velocity between phases.
- VGO cracking kinetics were modeled using a five-lump reaction scheme (converted VGO, light cycle oil or LCO, gasoline, light gases, and coke), as described in Section 4.2.2.

5. Conclusions

- (a) It is shown that a feedforward neural network (FNN) is valuable to reproduce the product distributions observed in the catalytic cracking experiments conducted using the CREC Riser Simulator.
- (b) It is proven that the resulting neural network model allows one to adjust the kinetic parameters of a five-lump model for FCC when using a dataset with limited experimental data.
- (c) It is demonstrated that the resulting kinetic model obtained with limited span kinetic parameters can be used in a 1D heterogeneous model for the simulation of an FCC riser industrial scale unit.
- (d) It is shown that the FCC riser industrial scale simulation provides valuable information about the optimization of VGO conversion and various product yields (light gases, gasoline, cycle oil, coke) in order to meet changing future energy market demands.

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Nomenclature

A	riser cross-sectional area (m^2)
C_i	molar concentration for i species (mol/m^3)
$C_{p,catalyst}$	specific heat capacity for the catalyst ($\text{kJ}/\text{kg}^\circ\text{C}$)
$C_{p,gas}$	specific heat capacity for the gas including hydrocarbons and steam ($\text{kJ}/\text{kg}^\circ\text{C}$)
D_o	effective diffusivity pre-exponential factor (m^2/s)

D_{Eff}	effective diffusivity (m^2/s)
E_D	energy of activation for VGO diffusional processes in zeolites (kJ/mol)
E_i	energy of activation for steps 1, 2, 3, 4 and 5 (kJ/mol)
$F_{catalyst}$	catalyst mass flow (kg/s)
F_{VGO_0}	flow of VGO fed to the industrial scale riser unit (kg/s)
F_t	total gas mass flow (kg/s)
h'_i	modified Thiele modulus (-)
k_4	kinetic constant for step 4. ($m^6/kg_{crystallite}mol_{hydrocarbon}s$)
k_{40}	kinetic constant pre-exponential factor for step 4 ($m^6/kg_{crystallite}mol_{hydrocarbon}s$)
k_i	kinetic constant for steps 1,2 and 3 ($m^6/kg_{crystallite}mol_{VGO}s$)
k_i	kinetic constant for steps 5 and 6 ($m^3/kg_{crystallite}s$)
k_{i0}	kinetic constant pre-exponential factor for steps 1,2, and 3 ($m^6/kg_{crystallite}mol_{VGO}s$)
k_{i0}	kinetic constant pre-exponential factor for steps 5 and 6 ($m^3/kg_{crystallite}s$)
L	characteristic dimension of the zeolite crystallite (m)
MW_i	molecular weight of A, B, C, D and E species (kg/kmol)
n	reaction order (-)
$Q_{cracking}$	heat consumed as a result of the cracking reaction (kJ/kg $_{crystallite}s$)
r_i	reaction rate for A, B, C, D, E species (mol/kg $_{crystallite}s$)
r_{mean}	average reaction rate (mol/kg $_{crystallite}s$)
t	reaction time (s)
T	temperature (K)
T_o	reference temperature for the kinetic modeling
U	superficial gas velocity in the riser (m/s)
V	CREC Riser Simulator reactor (m^3)
W_{cr}	crystallite weight in the FCC catalyst particle tested (kg)
W_i	weight of "i" product species in the CREC Riser Simulator runs (kg)
W_{VGO}	weight of VGO in the CREC Riser Simulator runs (kg)
$W_{VGO,0}$	initial weight of VGO in the CREC Riser Simulator runs ((kg)
X_E	coke over catalyst crystallite weight fraction ($kg_{coke}/kg_{crystallite}$)
X'_E	coke over VGO weight fraction (kg_{coke}/kg_{VGO})
X_{Ec}	maximum expected (critical) coke estimated at long reaction times, under the experimental conditions considered ($kg_{coke}/kg_{catalyst}$)
y_i	weight fractions for A, B, C and D (g of "i" hydrocarbons/g of VGO)
z	axial coordinate in riser simulator industrial unit (m)

Greek Symbols:

Δ_i	enthalpy of cracking steps 1, 2, 3, 4, 5 and 6 of the five-lump cracking model (kJ/kg)
ε	riser reactor void fraction (m^3_{void}/m^3_{total})
η_{ss}	effectiveness factor at steady state conditions (-)
φ	catalyst deactivating function (-)
γ	weight fraction of crystallite in the FCC catalyst = 0.3 ($g_{crystallite}/g_{catalyst}$)
λ	catalyst deactivating parameter (-)
$\rho_{catalyst}$	apparent catalyst density (g/cm 3)
ρ_{cr}	crystallite catalyst density (g/cm 3)
ν_i	stoichiometric coefficient for the formation of "i" product from VGO (-)

Subscripts:

A	designation for VGO
B	designation for cycle oil
C	designation for gasoline
D	designation for light gases
E	designation for coke
VGO	vacuum gas oil

Abbreviations:

AI	artificial intelligence
C/O	catalyst/VGO weight ratio
FCC	fluidized catalytic cracking

Appendix A. Simulation of an Industrial-Scale FCC Riser Unit

The simulation of an industrial FCC unit involves the simultaneous solution of the following lump balances and thermal balances, with new variables involved accounting for the flow of the riser unit such as: (a) Q the volumetric species flow, (b) F_{cr} the mass flow of crystallite in catalyst, (c) U the superficial gas velocity, and (d) F_{HC} the mass flow of VGO fed to the unit.

(a) Lump Species Balances

- For VGO

$$-\frac{Q}{F_{cr}}U\frac{dy_A}{dz} = \eta_{ss}\varphi\left(\frac{F_{HC}}{MW_AQ}\right)(k_1 + k_2 + k_3)y_A^2 \quad (A1)$$

- For Cycle Oil

$$\frac{Q}{F_{cr}}U\frac{dy_B}{dz} = \varphi\left[\eta_{ss}v_B\left(\frac{F_{HC}}{MW_AQ}\right)\left(\frac{MW_B}{MW_A}\right)k_1y_A^2 - k_5y_B\right] \quad (A2)$$

- For Gasoline

$$\frac{Q}{F_{cr}}U\frac{dy_C}{dz} = \varphi F\left[\eta_{ss}v_C\left(\frac{F_{HC}}{MW_AQ}\right)\left(\frac{MW_C}{MW_A}\right)k_2y_A^2 + \frac{v_C}{v_B}\left(\frac{MW_C}{MW_B}\right)k_5y_B - k_6y_C\right] \quad (A3)$$

- For Light Gases

$$\frac{Q}{F_{cr}}U\frac{dy_D}{dz} = \varphi\left[\eta_{ss}v_D\left(\frac{F_{HC}}{MW_AV}\right)\left(\frac{MW_D}{MW_A}\right)k_3y_A^2 + \frac{v_D}{v_C}\left(\frac{MW_D}{MW_C}\right)k_6y_C\right] \quad (A4)$$

- For Coke

$$\frac{Q}{F_{cr}}U\frac{dX_E'}{dz} = \varphi\left[\eta_{ss}v_E\left(\frac{F_{HC}}{MW_AV}\right)\left(\frac{MW_E}{MW_A}\right)k_4y_T^2\right] \quad (A5)$$

(b) Thermal Balance

$$\frac{dT}{dz} = -\frac{Q_{cracking}(1-\varepsilon)\gamma\rho_{catalyst}A}{(F_tC_{p,gas} + F_{catalyst}C_{p,catalyst})} \quad (A6)$$

with $Q_{cracking}$ being the combined heat of cracking accounting for the contribution of various steps in the reaction network as described in Table A1, $(1-\varepsilon)$ the volumetric concentration of catalysts, γ the crystallites weight fraction in the FCC catalyst, $\rho_{catalyst}$ the apparent catalyst density, F_t the combined mass flow of steam and hydrocarbons, $F_{catalyst}$ the catalyst mass flow, $C_{p,gas}$ the specific heat capacity for the combined steam and hydrocarbon, and $C_{p,catalyst}$ the specific heat capacity for the catalyst.

Appendix B. Thermodynamics of FCC in an FCC Riser Unit

The thermodynamics and the thermal parameters used in the 1D heterogenous model of Appendix A, as described using Equation (21), require a number of thermodynamics parameters, as reported in the following Table A1:

Table A1. Enthalpies of cracking and specific heat capacities.

$Q_{cracking}$ (kJ/kg _{crystallite} s)	$r_1\Delta H_1 + r_2\Delta H_2 + r_3\Delta H_3 + r_4\Delta H_4 + r_5\Delta H_5 + r_6\Delta H_6$
Step 1. A $\rightarrow$ B	$\Delta H_1 = 220$ kJ/kg
Step 2. A $\rightarrow$ C	$\Delta H_2 = 270$ kJ/kg
Step 3. A $\rightarrow$ D	$\Delta H_3 = 745$ kJ/kg

Table A1. Cont.

$Q_{cracking}$ (kJ/kg _{crystallite} s)	$r_1\Delta H_1 + r_2\Delta H_2 + r_3\Delta H_3 + r_4\Delta H_4 + r_5\Delta H_5 + r_6\Delta H_6$
Step 4. A → E	$\Delta H_4 = 820$ kJ/kg
Step 5. B → C	$\Delta H_5 = 50$ kJ/kg
Step 6. C → D	$\Delta H_6 = 475$ kJ/kg
Specific Heat Capacities	
$C_{p,catalyst}$	1.046 (kJ/kg°C)
$C_{p,gas}$	$\sum_1^4 y_i C_{p,i} + C_{p,steam} y_{steam}$ (J/kg°C)
$C_{p,i}$	3.430 (kJ/kg°C) for A, B, C, D
$C_{p,steam}$	$1937 = 0.9399 T + 0.0030 T^2 - 2.5329 \cdot 10^{-6} T^3 + 8.1785 \cdot 10^{-10} T^4$ (kJ/kg°C) with T in K

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