



Kinetic Parameters Estimation for Hydrocracker Reactor using Five Lumps Reaction Scheme

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ABSTRACT

The research study focused on kinetic parameters (pre-exponential factors and activation energies) estimation as a vital tool in solving the developed model equations of the hydrocracker reactor attached to the striping section of the modified modular refinery operations in Nigeria using five lump reaction path schemes. The estimation of these parameters are important as it gives best and most efficient values in comparison to experimental and literature data. Thus, these parameters are required in solving the developed model equations of the hydrocracker reactor. The principle of conservation of mass was applied in developing steady state models for packed bed catalytic hydrocracker reactor based on the evaluated isothermal nature of reaction taking place in the hydrocracker reactor. The kinetic parameters (pre-exponential factors and activation energies) for the five lump reaction scheme were evaluated using single point regression analysis with MATLAB software, and the results of pre-exponential factors for light ends, naphtha, diesel and bottom products were 51.9547hr^{-1} , $9.2999\text{E}8\text{hr}^{-1}$, $2.3399\text{E}16\text{hr}^{-1}$ and $2.25\text{E}8\text{hr}^{-1}$ respectively, while the estimated values of activation energy for light ends, naphtha, diesel and bottom products are 5.6151Kcal/mol , 41.3388Kcal/mol , 48.5074Kcal/mol and 23.5293Kcal/mol respectively. These results were compared with kinetic parameters experimental data of similar hydrocracker reactor study with percentage absolute error or minimum deviations within the allowable range. Therefore, these estimated kinetic parameters data are pertinent tools applied in solving the steady state models developed for hydrocracker reactor, thereby predicting the performance of the hydrocracker reactor with high efficiency or degree of accuracy.

KEYWORDS: Hydrocracker, Five Lump Scheme, Reaction Rate Constants, Pre-Exponential Factors, Activation Energies, Regression Analysis

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1. INTRODUCTION

Hydrocracking is a catalytic reaction process in the petroleum refineries for converting the higher boiling temperature residue such as the topping plant residue of crude oil into a lighter fraction of hydrocarbons such as gasoline, liquefied petroleum gas and diesel (Boosari *et al.*, 2017). Crude oil combines many different hydrocarbons, varying compositions, and complexities. To separate the crude oil into different components that make up the raw natural resource, crude oil must be refined (refinery process) so that components can be removed according to their temperature difference (Adeloye *et al.*, 2022). Parameter estimation therefore refers to the evaluation of the best values of critical parameters in a numerical model via assimilation of data or other similar methods. The procedure is thus effectively tried to resolve the deficiencies of the model as a result of parameter inaccuracy (Adeloye, 2022). Thus, estimation of parameter is the technique of assigning a parametric characteristic to an object, a physical



operation or measurements process that are determined from that object or operation (Mjalli & Ibrehem, 2011). Also, parameter estimation method reduces to deducing model parameters estimate that minimizes various residual error norm as various error norms leading to various data fit (Liang & Wu, 2008). Hence, evaluation of parameter and its deduction are important factor in developing models which depicts the process physical and chemical activities, thereby improving their models and optimize their operation (Mjalli & Ibrehem, 2011). Conservation equations that involve mass, momentum and energy balance expressions and constitutive laws (transport phenomena laws, Fourier's law of conduction etc. and chemical engineering are involved in modeling chemical processes. The efficiency of material balance analysis is dependent on the accuracy of data available and the extent to which the underlying assumptions are made (Adeloye *et al.*, 2016). The estimation of kinetic parameters in a developed model plays a vital role in model's simulation and validation, thereby improving the efficiency or accuracy of the developed models in describing the characteristics of the system. The assumed model consist of parameters in a finite region, whose results are determined by applying the methods of estimation. The main focus of modeling an engineering operation or process is performance improvement or process of design control, thereby leading to in-depth knowledge of a process' characteristics. These parameters usually define the system stability and behavioural control, thus parameter estimation from the process data is therefore an important operation in a system model analysis (Mejri *et al.*, 2018).

Different techniques have been applied in estimating kinetic parameters in general, which include simplex method for function minimization as a tool for kinetic parameters estimation of diesel

hydrotreating process by de Rochas *et al.* (2017) and optimization technique to obtain the best values of kinetic parameters in trickle-bed reactor process used for hydrodesulfurization of crude oil based on pilot plant experiment by Jarullah *et al.* (2011). Also, Sadeghi *et al.* (2010) and Elizalde *et al.* (2009) applied the continuous lumping model over different sets of measured data to minimize the least square error between the modeled and measured points and obtained a point estimate of the model parameters, and Kumar *et al.* (2009) applied hybrid particle swarm optimization to estimate the continuous lumping parameter values. However, there are associated uncertainties with these techniques based on parameters data that are unconsidered in the point estimation methods such as measurement errors, model structural error and operating conditions error. These are the main sources of uncertainty in the hydrocracking kinetic models that affects kinetic parameters estimation. These uncertainties are addressed in this study via the single point regression analysis with MATLAB software on the experimental kinetic values based on error minimization.

Furthermore, the advantages of developing kinetic models by chemical engineers with accurate determination of parameters are of great importance due to control strategies development and optimization of the process based on fundamental operational models. Kinetic characteristics are deduced accurately based on experimental analysis and the estimated model data applied should match with the experimental data, plant data or literature data effectively, thereby minimizing errors among experimental, plant, literature and theoretical data (Poyton *et al.*, 2006). Thus, in this research study, a hydrocracker reactor model was developed for processing 30,000bpd capacity modular refinery (topping plant) residue or bottom product for kinetic parameters (pre-



exponential factors and activation energies) estimation of the hydrocracker reactor attached to the stripping section of the modified modular refinery operations in Nigeria using five lump reaction path schemes (Adeloye *et al.*, 2022). The objectives of the study was achieved by evaluating the voidage value, evaluation of the rate equation, development of model equations for predicting the performance of the hydrocracker, estimation of kinetic parameters such as pre-exponential factors and activation energies of the hydrocracking reactor using regression analysis with MATLAB software, comparison of hydrocracker estimated kinetic parameters with experimental data or plant data to check for absolute value error or deviation and efficiency of estimated data and comparison of developed model yield and Aspen HYSYS yield of the hydrocracker.

2. MATERIALS AND METHODS

The major materials used in this research study include conventional modular refinery residue and hydrocracker reactor unit with five lump reaction schemes occurring. The methods applied are highlighted thus.

2.1 Nature of Reaction in Hydrocracking Reactor

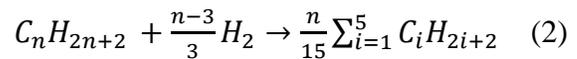
The nature of the reaction occurring in the hydrocracking reactor was determined from its voidage value as described by Adeloye, 2022.

$$\varepsilon = \frac{V_{XA=1} - V_{XA=0}}{V_{XA=0}} \quad (1)$$

The sum of the coefficient of stoichiometry of the reactants and products are obtained from the balance chemical equation for each reaction.

Besides, hydrocracking reactor is used for breaking of heavy hydrocarbon (crude distillation unit residue) into a more favourable light product. This reactor is designed for treating topping plant

residue (bottom product), and the general hydrocracking reaction of higher paraffins to lower hydrocarbon as expressed by Hill *et al.* (2007) and Akpa and Adeloye (2017).



2.2 Kinetics of the Reaction

A kinetic model equation is an important scheme for design adequacy and solution of chemical operations (Cao *et al.*, 2020). The reaction kinetics therefore refers to the equation of rate and rate constant of the reaction occurring in the hydrocracking reactor. Thus, in this study, five lumps scheme which include the feedstock (conventional modular refinery residue or bottom product at 370°C, specific gravity 15.6°C, molecular weight of 463.06 and Watson characterization factor of 12.71), and products from hydrocracker that include light ends (liquefied petroleum gas), naphtha, diesel and bottom are used in developing models of the reactor. The reaction pathway for the hydrocracking process for five lumps scheme as described by Adeloye (2022) is shown in Figure 1. Therefore, a single stage fixed bed catalytic hydrocracker reactor of capacity 10,000bpd operating at a pressure of 183bar (150-200bar) and temperature of 380°C (300-425°C) was applied in this study owing to the light and medium sweet Nigerian crude oil types as described by Adeloye *et al.* (2022) for conversion of 380.3254Kgmol/hr. (9127.8096Kgmol/day) modular refinery residue to more valuable products. The composition of the conventional modular refinery residue (feedstock) into the hydrocracker reactor is shown in Table 1.

Table 1: Properties of Feedstock

Properties	Value
Specific Gravity @ 15.6 ⁰ C	0.908
Feed Flow Rate (kgmol/day)	9127.8096
Pressure (bar)	183
Temperature (⁰ C)	380
Molecular Weight	463.06
Mass Density (Kg/m ³)	650.93
Watson Factor	12.71

(Adeloye, 2022)

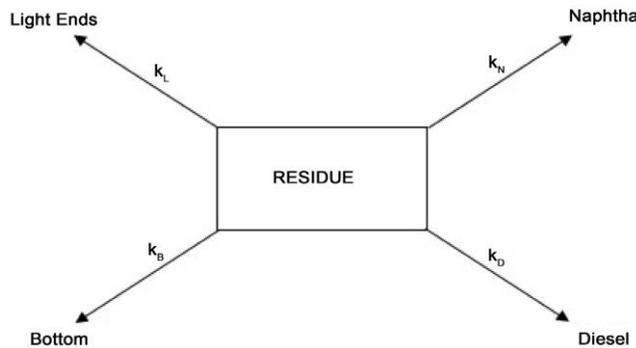


Fig 1: Five Lumps Reaction Scheme (Adeloye, 2022)

The five lumps scheme applied in this study include residue, light ends, naphtha, diesel, bottom product and their rate equations determined and respective rate constant described by Arrhenius equation.

i. Feedstock

Based on the reaction lumping path in Figure 1, the rate of reaction for the feedstock (residue) in terms of mass fraction is expressed as

$$-r_R = -(k_L y_L + k_N y_N + k_D y_D + k_B y_B) \eta \quad (3)$$

ii. Light Ends Product

The rate equation for the production of light end in terms of mass fraction is described thus

$$-r_L = -k_L y_L \eta \quad (4)$$

iii. Naphtha Product

The hydrocracking product (naphtha) rate equation in terms of mass fraction is expressed as

$$-r_N = -k_N y_N \eta \quad (5)$$

iv. Diesel Product

The reaction rate equation describing the production of diesel by hydrocracking process is expressed in terms of mass fraction

$$-r_D = -k_D y_D \eta \quad (6)$$

v. Bottom Product

The rate equation for the production of bottom product in the hydrocracking of feedstock in terms of mass fraction

$$-r_B = -k_B y_B \eta \quad (7)$$

In addition, the reaction rate constants for the conversion of feedstock and production of light end, naphtha, diesel and bottom products can be evaluated from Arrhenius equation.

$$k_i = k_0 \exp\left(\frac{-E_i}{RT}\right) \quad (8)$$

Therefore, writing the reaction rate constants for respective reaction path of the five lump scheme yields

i. Light Ends

$$k_L = k_{L0} \exp\left(\frac{-E_L}{RT}\right) \quad (9)$$

ii. Naphtha

$$k_N = k_{N0} \exp\left(\frac{-E_N}{RT}\right) \quad (10)$$

iii. Diesel

$$k_D = k_{D0} \exp\left(\frac{-E_D}{RT}\right) \quad (11)$$

iv. **Bottom**

$$k_B = k_{B0} \exp\left(\frac{-E_B}{RT}\right) \quad (12)$$

2.3 Development of Model Equations for Hydrocracker Reactor

A schematic flow diagram of catalytic hydrocracker (packed bed) reactor is shown in Figure 2

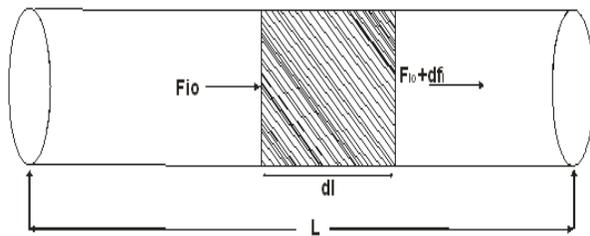


Fig 2: Packed Bed Catalytic Hydrocracker Reactor

The following assumptions are applied in developing model equations that predicts the performance of catalytic hydrocracker reactor.

- i. The rate of hydrocracking does not depend on hydrogen concentrations and there is excess availability of hydrogen gas in the process. This assumption is in tandem with other previous studies by Adeloye and Igbagara (2022), Farag *et al.* (2016), Sadighi (2013) and Mohanty *et al.* (1991).
- ii. The reaction rate does not depend on hydrogen gas partial pressure.
- iii. The feedstock and all products are in the liquid phase and hydrogen feed is pure.
- iv. The reaction paths of the hydrocracking reaction process is first order reaction.

The general material balance equation is expressed as thus.

$$\begin{aligned} & \text{Rate of accumulation of material into the reactor} \\ & = \text{Rate of inflow into the reactor} \\ & - \text{Rate of outflow from the reactor} \\ & \pm \text{Rate of prod. or depletion within the reactor due} \\ & \text{to chemical rxn} \end{aligned} \quad (13)$$

Defining each term in Equation 13 at steady state process,

$$\text{Rate of Accumulation of Material into the Reactor} = 0$$

$$\text{Rate of Inflow into the Reactor} = v_0 \rho_i$$

$$\begin{aligned} \text{Rate of Outflow from the Reactor} \\ = v_0 (\rho_i + d\rho_i) \end{aligned}$$

$$\text{Rate of Depletion within the Reactor due to Chemical Reaction} = \rho_{gR} \varepsilon (-r_i) dV$$

Therefore, the change in mass fraction of specie (feedstock and products) in terms of hydrocracker reactor dimensionless length is expressed as

$$\frac{dy_i}{dl_d} = -\tau \varepsilon (-r_i) \quad (14)$$

Hence, writing Equation 14 for the five lump scheme yields

i. **Feedstock**

$$\begin{aligned} \frac{dy_R}{dl_d} = & -\tau \eta \varepsilon \left(k_{L0} \exp\left(\frac{-E_L}{RT}\right) y_L + \right. \\ & k_{N0} \exp\left(\frac{-E_N}{RT}\right) y_N + k_{D0} \exp\left(\frac{-E_D}{RT}\right) y_D + \\ & \left. k_{B0} \exp\left(\frac{-E_B}{RT}\right) y_B \right) \end{aligned} \quad (15)$$

ii. **Light Ends**

$$\frac{dy_L}{dl_d} = \tau \eta \varepsilon k_{L0} \exp\left(\frac{-E_L}{RT}\right) y_L \quad (16)$$

**iii. Naphtha**

$$\frac{dy_N}{dl_d} = \tau \varepsilon \eta k_{NO} \text{Exp} \left(\frac{-E_N}{RT} \right) y_N \quad (17)$$

iv. Diesel

$$\frac{dy_D}{dl_d} = \tau \varepsilon \eta k_{DO} \text{Exp} \left(\frac{-E_D}{RT} \right) y_D \quad (18)$$

v. Bottom

$$\frac{dy_B}{dl_d} = \tau \varepsilon \eta k_{BO} \text{Exp} \left(\frac{-E_B}{RT} \right) y_B \quad (19)$$

2.4 Estimation of Kinetic Parameters

The kinetic parameters or characteristics such as pre-exponential factors and activation energies are useful in evaluating the rate constants applied in solving the developed model equations for the hydrocracker reactor. These parameters are estimated in this study by applying the single point regression analysis and MATLAB software that solves complex non-linear expressions, and the estimated values are considered to be the best values among plant data, literature data, and experimental data in solving developed model equations. Thus, these kinetic parameters are estimated by minimizing the objective function, S; subject to the constraint $y_{i,0}$, that gives the estimated values of $y_{i,est}$ as:

Objective function:

$$S = \sum_{i=1}^m (y_{i,Plant} - y_{i,Cal})^2 \quad (20)$$

Subject to (Constraint) models $y_{i,lit}$ such that $y_{i,lit} > 0$

The incremental change Δs was obtained as:

$$\Delta s = -[[n * p][p * n]]^{-1}[n * p] \quad (21)$$

Therefore, estimation model for kinetic parameters (pre-exponential factors and activation energies) are expressed in Equations 22 and 23 respectively

$$k_{i0}^{(j+1)} = k_{i0}^j + \alpha \Delta s \quad (22)$$

$$E_i^{(j+1)} = E_i^j + \alpha \Delta s \quad (23)$$

The criteria for convergence is expressed as

$$F_{cal} \geq F_{tab}$$

If $F_{cal} \geq F_{tab}$, stop iteration and compute the results which are the kinetic parameters obtained, otherwise continue iteration till $F_{cal} \geq F_{tab}$

$$\text{Also, } F_{cal} = \frac{MSM}{MSE}$$

where, MSM is mean of square mean = $\frac{\text{Sum of Square Mean}}{P\text{-Components}}$,

MSE is mean of Square Error = $\frac{\text{Sum of Square Error}}{(n-p) \Rightarrow \text{Degree of Freedom}}$, and F_{tab} is deduced at 95% confidence level.

The estimated rate constant values for the five lump system are evaluated using Equations 9, 10, 11 and 12 respectively.

2.4.1 Kinetic Parameters Estimation Procedures

The single point regression technique is useful in the determination of kinetic parameters (activation energies and pre-exponential factors) for the hydrocracker five lump model. The procedures or steps involved in hydrocracker kinetic parameters estimation are discussed thus.

Step 1: Steady state model yield fractions (Equations 16, 17, 18 and 19) are solved numerically with MATLAB software

Step 2: Simulated yield fractions are compared with Aspen HYSYS yield fractions to estimate percentage deviations.

Step 3: Steady state yield fractions of the products are then subjected to estimation process:



The objective function (S) for the estimation technique is expressed as:

$$S = \sum_{i=1}^4 \{(y_{iPlant} - y_{iCal})^2\}$$

Subject to (Constrain functions) given as:

$$y_{L0} = 0.3435; y_{N0} = 0.1081; y_{D0} = 0.3149; y_{B0} = 0.2336; T = 653K$$

$$y_{i,0} > 0; i = L, N, D, B$$

$y_{i,cal}$ is computed from MatLab software

The statistical test approach, that is F_{cal} as the convergence or limit of boundary for the iteration estimation operation is step-wisely stated as follows

i. $y_{i,plant}$ is obtained from Aspen Hysys result or initial boundary conditions

ii. \bar{y}_i is mean value of y_i , that is $\bar{y}_i = \frac{\sum y_i}{n}$; $n = 27$

iii. Sum of Residual Errors (SSE) computation

$$SSE = \sum_{i=1}^4 (y_{iPlant} - y_{iCal})^2$$

iv. Sum of Square Mean (SSM) computation

$$SSM = \sum_{i=1}^4 (y_{iPlant} - \bar{y}_{iCal})^2$$

v. Compute F_{cal}

$$F_{cal} = \frac{\frac{SSM}{P}}{\frac{SSE}{n-p}} = \frac{MSM}{MSE}$$

Mean of Square Mean (MSM) = $\frac{SSM}{P}$ and Mean of

$$\text{Square Error (MSE)} = \frac{SSE}{n-p}$$

where, p is the number of kinetic parameters to be evaluated and n is number of points or experimental results obtained from simulation.

Compute F_{tab} from 5% confidence level (t_{α})

$$1 - t_{\alpha} = 1 - 0.05 = 0.95$$

vi. Degree of freedom of Error (DFE) = $n - p$

vii. Corrected degree of freedom (DFM) computation

$$DFM = P - 1$$

af

$$= (1 - \alpha, p - 1, n - p) \text{ such that } qf(0.95, 3, 23) \text{ for } n = 27, p = 4$$

F_{tab} is deduced from table of F - test on range (3,23) at 95% confidence level.

viii. Choose α such that $0 < \alpha < 1$

$$\alpha = 0.85$$

ix. Compute for new activation energies and pre-exponential factors

$$E_i^{j+1} = E_i^j + \alpha \Delta s$$

$$k_{i0}^{j+1} = k_{i0}^j + \alpha \Delta s$$

where $\Delta s(\text{increment}) = -(J_r J_r^T)^{-1} J_r$,

J_r is matrix of $(n \times p)$,

J_r^T is transpose of J_r matrix $(p \times n)$

Therefore $\Delta s = -[(n * p)(p * n)]^{-1}(n * p)$

x. From the table of F-test, F_{tab} is determined as:

At 95% confidence level $F_{tab} = 2.278$

xi. Termination criteria

If $F_{Cal} \geq F_{tab}$, stop iteration and the E_i and K_{i0} values are determined, else continues till $F_{Cal} \geq F_{tab}$

- xii. The estimated values of E_i and K_{i0} obtained are applied in estimating the optimal rate constants, k_i

$$k_i = k_{i,0} \exp\left(\frac{-E_i}{RT}\right)$$

$$i = L, N, D, B$$

Step 4: The deduced rate constant values obtained are used to get optimal yield fractions of the products and feedstock depletion.

In addition, the kinetic parameters values applied in this study is based on experimental analysis carried out by Sadighi (2013) as shown in Table 2

Table 2: Five Lumps Kinetic Parameters

Parameters	Light Ends	Naphtha	Diesel	Bottom
Activation Energy (Kcal/mol)	5.61	41.34	49.63	23.51
Pre-Exponential Factor (hr ⁻¹)	52.84	9.3E8	2.34E16	2.25E8

(Sadighi, 2013)

3 RESULTS AND DISCUSSION

3.1 Nature of Reaction

The nature of hydrocracker reactor is determined by evaluating the reaction taking place in the reactor through the application of Equation 1 and this evaluation analysis of hydrocracker reactor yielded the voidage value of zero, which shows that hydrocracker reactor operational process is an isothermal operation and this is in tandem with other researches or studies on hydrocracker reactor by Matos and Gurirardello (2000) and USEIA (2013). Thus, this deduction is applied in developing models for the hydrocracker reactor.

Table 3: Comparison of Pre-Exponential Factors

Activation Energy (E_i)	Experimental Data (Sadighi, 2013)	Estimated Data	Deviation (%)
Light Ends	5.61	5.6151	0.0909
Naphtha	41.34	41.3388	0.0029
Diesel	49.63	48.5074	2.2619
Bottom	23.51	23.5293	0.0820

3.2 Kinetic Parameters Validation

The results of the estimated hydrocracker reactor kinetic parameters (pre-exponential constants and activation energies) of the five lump reaction schemes are compared with kinetic parameters experimental result for hydrocracker by Sadighi (2013) in checking the accuracy of estimated kinetic parameters. Therefore, the comparison of experimental data and estimated results of pre-exponential factors and activation energies for the five lump schemes are highlighted in Tables 3 and 4 respectively.

The results of the estimated pre-exponential factors of the five lump schemes evaluated in this study were compared with experimental pre-exponential factors for five lump schemes by Sadighi (2013). The percentage deviation or absolute error values between the research study and experimental pre-exponential factors are minimal with 1% as maximum percentage deviation for light ends pre-exponential factors, while other deviations for pre-exponential factors are extremely below 1%.

Furthermore, the estimated results of activation energies for the five lump schemes were also compared with the experimental results of activation energies for five lump schemes carried out by Sadighi (2013) as shown in Table 3. The comparison yielded percentage absolute error value of 2.2% maximum for distillate activation energy



while other products deviations are quite negligible, which refers to the accuracy or correctness of the estimated activation energies.

Table 4: Comparison of Activation Energy Data

Parameters	Aspen HYSYS Yield	Model Yield	Deviation (%)
Light Ends	0.3435	0.3588	4.4542
(Gases)	0.1081	0.1135	4.9954
Naphtha	0.4316	0.4403	2.0158
Diesel	0.1168	0.0874	25.1712
Bottom			

3.3 Hydrocracker Reactor Models Validation

The developed model equations of hydrocracker for processing the topping plant residue yielded a first order ordinary differential equations as depicted in Equations 15, 16, 17, 18 and 19 respectively, which were solved using fourth order Runge-Kutta algorithm in MATLAB ODE45 solver. The developed model results were compared with Aspen HYSYS hydrocracker reactor simulated results of Okoro (2012) as shown in Table 5.

Table 5: Comparison of Aspen HYSYS and Developed Models Yield of Hydrocracker

Pre-Exponential Factors (k_{i0})	Experimental Data (Sadighi, 2013)	Estimated Data	Deviation (%)
Light Ends	52.84	51.9547	1.6754
Naphtha	9.3E8	9.2999E8	0.00108
Diesel	2.34E16	2.3399E16	0.00427
Bottom	2.25E8	2.2500E8	0.0000

The comparison of products yield of hydrocracker reactor using Okoro (2012) residue as feedstock from Aspen HYSYS and developed models

showed minimal error or deviation value, thereby verifying the closeness or accuracy of the estimated kinetic parameters and predicted models. Thus, based on the efficient kinetic parameters' values, these model equations can be applied in simulating and predicting the performance of the hydrocracker reactor.

4. CONCLUSION

This research study focused on estimation of kinetic parameters such as pre-exponential factors, activation energies and rate constants for five lump reaction paths, which are important tools in solving and simulating the predicted or developed models for the hydrocracker reactor. In achieving the study's aim, some objectives were highlighted and achieved that included the evaluation of the nature of reaction occurring in the hydrocracker reactor via its voidage value as isothermal based on operational process (reaction) taking place in the reactor. In addition, the reaction kinetic parameters such as pre-exponential factors, activation energies and rate constants were estimated using single point regression analysis with MATLAB software.

The evaluated kinetic parameters were compared with experimental results of kinetic parameters of similar hydrocracker study with the percentage deviation or absolute error less than 1%. Thus, the values of these kinetic parameters were applied in solving the developed models of the hydrocracker reactor from the first principle, thereby predicting feedstock (residue) depletion and products (light ends, naphtha, diesel and bottom) yield of the hydrocracker, which were compared with Aspen HYSYS software hydrocracker yields.

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y_B	Mass Fraction of Bottom	
η	Catalyst Effectiveness Factor	Percent
k_i	Reaction Rate Constant of Specie i	hr ⁻¹
k_0	Pre-Exponential Constant	hr ⁻¹
E_i	Activation Energy of Specie i	kcal/mol
T	Temperature in Kelvin	K
R	Universal Gas Constant	kcal/molK

NOMENCLATURES

Symbols	Definition	Units
ε	Voidage Value	
$V_{XA=0}$	Sum of Reactant Stoichiometric Coefficients	
$V_{XA=1}$	Sum of Product Stoichiometric Coefficients	
k_L	Rate Constant for Light Ends	hr ⁻¹
y_L	Mass Fraction of Light Ends	
k_N	Rate Constant for Naphtha	hr ⁻¹
y_N	Mass Fraction of Naphtha	
k_D	Rate Constant for Diesel	hr ⁻¹
y_D	Mass Fraction of Diesel	
k_B	Rate Constant for Bottom	hr ⁻¹

CONFLICTS OF INTEREST

The authors declare no conflicts of interest regarding the publication of this research paper.