Computational Fluid Dynamic Modeling and Simulation of Hydrocracking of Vacuum Gas Oil in a Fixed-Bed Reactor

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ABSTRACT: A four-lump computational fluid dynamic (CFD) model was proposed for the investigation of vacuum gas oil hydrocracking in a trickle-bed reactor. The experiment was conducted at 360−390 °C and 146 bar in the reactor at three different flow rates. It was found that the modeling predictions of vacuum gas oil cracking agreed well with the experimental measurements. Furthermore, the developed model analyzed the effects of the feed flow rate in the reactors on the concentration distribution and product yield. The maximum yields of the products including distillate (31%), naphtha (14%), and gas (3%) were obtained at the lowest feed flow rate. However, the feed flow rate enhancement from 0.1568 to 0.2059 kg·h⁻¹ led to the increasing feed concentration and reducing the product concentration at the outlet of the reactor. The latter phenomenon was happened due to the decreasing feed residence time with the increasing mass flow rate.

1. INTRODUCTION

Rising energy demand with the lack of abundant light crude oil resources has forced the researchers to pay much more attention to use widely available heavy crude oil. However, the use of cutting-edge technologies is required for upgrading the oil properties because of the low quality as well as the difficulties in transporting heavy oil. Hydrocracking as a refining process is usually considered the most efficient technique to convert heavy fractions in heavy crude oil into valuable products like naphtha. Various kind of reactors including fixed-bed, moving-bed, ebullated-bed and slurry bed reactors can be used in the hydrocracking process in which the type of reactor depends on the conversion level and the amount of metals and asphaltenes in the heavy crude oil. Catalyst deactivation during hydrocracking, deposition of coke, and formation of sludge in the product are the main operational problems in the hydrocracking process. Experiments to find optimum operational conditions, catalyst preparation, and kinetic investigations are expensive and time-consuming. An attractive alternative way to decrease the cost and save time is the development of mathematical models that sufficiently explain the behavior of the process. However, mathematical analysis of the hydrocracking process of heavy crude oil is too difficult because of the association of many parameters including complex reaction mechanisms, porous medium, many components, mass and heat transport phenomena, etc. The reaction kinetics is one of the major parameters that deserves careful attention to obtain a reliable reactor model. Classification of the components into a few equivalent groups can be considered to make the problem simple. This approach is named the lumping method, assuming that each group is an independent entity. A multiphase reactor associated with heavy oil hydrocracking was prosperously modeled taking into account the influences of both radial/axial dispersions. It was found that the axial-dispersion model can be used to interpret the system for dynamic and steady-state implementations with good accuracy. Zhong et al. optimized the hydrocracking process on the basis of the Kriging surrogate method, and an optimization algorithm was developed to optimize the process’s operational conditions. The developed optimization algorithm integrated both the adaptive step-size global and local search strategy to minimize the predictor.

The lump first-order kinetics was used to study the efficiency of a residue hydrotreater, and the residue was classified into two lumps including “easy” and “hard” cracks. The lumped method was also implemented by Aboul-Gheit to predict the...
vacuum gas oil (VGO) hydrocracking, explaining the composition in molar concentrations. A four-lump kinetic model consisting of hydrogen consumption for VGO hydrocracking in a pilot-plant reactor was developed in one dimension (1D) and two dimensions (2D). The hydrocracking reactor was well perceived as a plug flow reactor and modeled by the cellular network approach. The development of the 2D model was reported by the solution of mass and momentum conservation equations in the reactor. The model’s findings revealed that the developed model could be used to enhance the accuracy of the efficiency prediction compared to that of the one-dimensional model. Sanchez et al. investigated the development of a kinetic model for heavy oil hydrocracking including five lumps. Prediction of kinetic parameters was done from measured data achieved in a fixed-bed reactor applying Maya heavy crude oil.

Computational fluid dynamics (CFD) now plays a vital role in analyzing the hydrodynamics and reaction kinetics of the multiphase systems with the development of computational technology. It was applied to predict the performance of the pulsing flow in trickle-bed reactors. Eulerian-based CFD computations have been able to appropriately handle the experimental data collected on pulsing flow circumstances for both bulk temperature and normalized species concentration. Also, the technique was implemented to calculate the local heat transfer coefficient, which is regarded as a momentous parameter in the computation of energy transfer between the fluid and the particle in packed-bed reactors.

The objective of the current work is to extend the studies by Sadighi et al. to investigate the hydrodynamics, reaction kinetics, and influence of operational parameters on the reactor performance by applying a comprehensive CFD model via COMSOL package.

### 2. EXPERIMENTAL SECTION

In this work, hydrotreating and hydrocracking of the VGO were conducted in a pilot-plant reactor at high pressure. A cylindrical fixed-bed reactor with an internal diameter of 16 mm and a height of 1220 mm was used for the experiments. The bottom and the top of the bed were filled with inert SiC particles with a diameter of 0.1 m to make sure there is even liquid and gas distribution in the reactor. Hydrocracking catalysts were packed on the SiC particles and then the hydrotreating catalysts were placed on the top of the hydrocracking catalysts. The details of the experiments can be found in our previous papers. The operating conditions are provided in Table 1.

### 3. MODEL DEVELOPMENT

A four-lump mathematical model consisting of distillate, vacuum gas oil, naphtha, and gas partitions was used to determine their concentration distribution and conversion along the length of the reactor. The four-lump model was selected due to considerable instrumental error when the higher amount of products was considered. Moreover, increment in the number of lumps will increase the number of model coefficients (activation energy and frequency factor), which consequently results in increasing the degree of freedom and uncertainty of the model.

First, the vacuum gas oil is converted to distillate, naphtha, and gas; then, distillate reacts with the catalyst surface for the production of the naphtha and gas. Finally, the gas can be also generated by naphtha. The hydrogen consumption is neglected in this combined bed model. It should be pointed out that during the hydrotreating and hydrocracking chemical reactions, H₂ molecules are absorbed in the hydrocarbon structure but sulfur and nitrogen are eliminated. Only 1% error in the mass balance was observed by making this assumption.

A schematic demonstration of the modeled pilot-scale reactor is given in Figure 1. As can be seen, the first step of hydrocracking consists of mixing the VGO and H₂ prior to their entrance to the reactor. Then, the feed enters the vessel’s bottom at low velocity, and the chemical reactions occur as the feed passes inside the porous section of the reactor. The reaction blend including unreacted feed and products leaves the reactor. Hence, the reactor includes three compartments: the bottom free side, the porous medium, and the top free side. The steady-state two-dimensional mass balance is implemented in the porous section of the reactor. The mathematical model is developed based on the simplifying assumptions listed below; more information can be found in our previous papers.

1. Steady-state and isothermal modes.
2. Pure hydrogen was used.
3. Carrying out a first-order hydrocracking reaction in the presence of excess H₂ in which the hydrocracking reactions are not dependent on the H₂ concentration.
4. Void distribution is even inside the bed.
5. The gas—liquid intraphase exchanges are ignored.
6. Sulphur/metal toxicity, coke deposition, sintering, and active surface loss are not involved in the model.

### 3.1. Mass Transfer Equation

To develop the reactor’s model, the transport of diluted species in the porous media is applied to predict the concentration and transport of different parameters values unit

| parameters                   | values | unit |
|------------------------------|--------|------|
| the percentage of the fresh feed | 87     | %    |
| the percentage of the recycle feed | 13     | %    |
| liquid hourly space velocity (LHSV) | 0.8, 0.9, 1.05 | h⁻¹ |
| temperature                  | 360–390 | °C   |
| pressure                     | 146    | bar  |

Figure 1. Schematic illustration of the hydrocracking process in the bed reactor.
Table 2. Developed Model Inputs for the Hydrocracking Process in the Fixed-Bed Reactor²⁹

| properties                              | values  | unit   |
|----------------------------------------|---------|--------|
| feed density                           | 890.31  | kg·m⁻³ |
| catalyst porosity                      | 0.35    |        |
| permeability                           | 1.00 × 10⁻¹² | m²⁻¹  |
| feed mass flow                         | 0.1568 (LHSV = 0.8 h⁻¹) | kg·h⁻¹ |
| operating temperature                  | 663.15  | K      |
| operating pressure                     | 146     | bar    |
| feed velocity                          | 0.0003769 | m·s⁻¹  |
| length of the catalyst bed             | 1.22    | m      |
| diffusion coefficient of feed          | 1.64284 × 10⁻¹⁰ | m²·s⁻¹ |
| diffusion coefficient of distillate    | 1.76658 × 10⁻¹⁰ | m²·s⁻¹ |
| diffusion coefficient of naphtha       | 1.77461 × 10⁻¹⁰ | m²·s⁻¹ |
| diffusion coefficient of gas           | 4.84921 × 10⁻¹² | m²·s⁻¹ |
| molecular weight of feed               | 420     | kg·mol⁻¹|
| molecular weight of distillate         | 220.3   | kg·mol⁻¹|
| molecular weight of naphtha            | 113.8   | kg·mol⁻¹|
| molecular weight of gas                | 38      | kg·mol⁻¹|
| initial concentration of feed          | 890.31  | kg      |
| final concentration of feed            | 736.98  | kg      |
| initial concentration of distillate     | 0       | kg      |
| final concentration of distillate       | 69.968  | kg      |
| initial concentration of naphtha        | 0       | kg      |
| final concentration of naphtha          | 0       | kg      |
| initial concentration of gas            | 28.48   | kg      |
| final concentration of gas              | 6.258   | kg      |

components in both regions, i.e., free and porous media. It involves reaction term and solute sources for modeling solute transport:

\[
\frac{\partial (\theta c_i)}{\partial t} + \frac{\partial (\rho c_i \epsilon)}{\partial t} + \nabla \cdot u \nabla c_i = R_i + S_i
\]  

(1)

\[J_i = -\theta D_{i,j} \nabla c_i\]  

(2)

\[\theta = \frac{\epsilon_p}{r}\]  

(3)

\[D_{i,j} = \frac{\epsilon_p D_{F,i}}{r}\]  

(4)

It can be written in steady-state condition and \(S_i = 0\) as follows:

\[\nabla \cdot u \nabla c_i = R_i + S_i\]  

(5)

\[
\frac{\tau D_{i,j}}{\epsilon_p} \left[ \frac{\partial^2 c_i}{\partial r^2} + \frac{1}{r} \frac{\partial c_i}{\partial r} + \frac{\partial^2 c_i}{\partial z^2} \right] = u \frac{\partial c_i}{\partial z} - \eta (1 - \epsilon_p) R_i
\]  

(6)

where \(i\) is either fresh feed (F) or gas (G); \(c\) is the concentration of the reactants or the products; \(\eta\) is the effectiveness factor that is 0.7 for a cylindrical catalyst in a trickle-bed regime;²⁸ and \(D_{i,j}\) is the effective diffusivity of the components. \(R_i\) expresses the reaction term (mol·m⁻³·s⁻¹). The velocity parameter can be expressed analytically or through coupling a momentum transfer to the mass transfer equation. The distribution of the velocity vector is achieved by the numerical solution of the momentum equation in a porous medium, i.e., the Brinkman equation. Hence, the continuity and momentum equations should be coupled and properly solved at the same time to determine the concentration distribution of the reactant and products.

Diffusivity of the feed and products was computed using the Wilke–Chang equation:

\[D_i = 7.4 \times 10^{-8} \sqrt{\frac{\rho MT}{\mu v_i^{0.6}}}\]  

(7)

Figure 2. Change in porosity function according random in different parts of the reactor.
where \( v \) (cm\(^3\)-g mole\(^{-1}\)) and \( M \) denote the molar volume and the molecular weight of the chemicals, respectively. Also, the viscosity of the bulk stream (\( \mu \)) must be defined as centipoise (cp) to achieve the diffusion coefficient in cm\(^2\)-s\(^{-1}\). The equation for determining the rate of feed consumption and products formation in the reactor based on selected four-lump model can be written as follows

\[
R_{vgo} = -(k_{1vgo} + k_{2vgo} + k_{3vgo})
\]  
(8)

\[
R_{dis} = k_{1dis} - k_{2dis} - k_{3dis}
\]  
(9)

\[
R_{naph} = k_{1naph} + k_{2naph} - k_{3naph}
\]  
(10)

\[
R_{gas} = k_{1gas} + k_{2gas} + k_{3gas}
\]  
(11)

The boundary conditions for the mass transfer are expressed as follows:

- \( r = 0, z = L_z \), axial symmetry
- \( r = R_z, z = L_z \), no flux
- \( r = R_z, z = 0 \), inflow, \( C_{vgo} = C_{naph} = C_{dis} = 0, C_{gas} = 0 \)
- \( r = R_z, z = L_z \), outlet, pressure = 146 bar

To take into account the porosity of the catalyst, random variations in porosity versus those in \( r \) and \( z \)-directions are generated. Then, a multivariable function is developed in which porosity and \( r \) values along \( r \) and \( z \)-directions are depicted in Figure 2.

3.2. Momentum Transfer Equation. The Brinkman equations are normally used for the simulation of transport in the porous media and are utilized in this study. It was used for simulating high-velocity fluid motion in the porous system with the kinetic potential from fluid motion, pressure, and gravity driving the fluid flow. They extend Darcy’s model to interpret the kinetic energy dissipation by viscous shear, the same as the Navier–Stokes equations. Hence, the Brinkman model is appropriately developed for modeling a rapid flow in porous media, consisting of transitions between the slow-moving fluid in porous media determined by Darcy’s law and fast-moving fluid in channels explained by the Navier–Stokes equations. The Brinkman equations interface calculates both the pressure and the velocity

\[
\nabla \cdot (-pI + K) = \left( \mu k^{-1} + \beta l \right) I + \frac{Q_m}{\varepsilon_p} + F
\]  
(12)

\[
\nabla \cdot \left( \frac{1}{\varepsilon_p} I \right) = Q_m
\]  
(13)

\[
K = \mu - \frac{1}{3} \nabla (\nabla u + (\nabla u)^T) - \frac{2}{3} \mu \frac{1}{\varepsilon_p} I
\]  
(14)

In this equation, \( p, I, K, \mu, \beta l, \varepsilon_p \) and \( F \) are the pressure of fluid, identity tensor, permeability coefficient, viscosity of the fluid, Forchheimer coefficient, porosity, and body force, respectively.

Consequently, the boundary conditions associated with momentum transfer are represented as follows

- \( r = 0, z = L_z \), axial symmetry
- \( r = R_z, z = L_z \), wall, no slip
- \( r = R_z, z = 0 \), inlet, \( u = u_0 \)
- \( r = R_z, z = L_z \), outlet, pressure = 146 bar

4. RESULTS AND DISCUSSION

4.1. Model Validation. The yields of gas, naphtha, distillate, and residue, which is expressed as the ratio of a lump to total values of all lump, was used to compare the experimental data with the obtained results from the developed model. The comparison of the experimental data with the modeling results is shown in Figure 3. The average absolute value of the relative error for the prediction of the yields of gas, naphtha, distillate, and residue using the proposed model was obtained to be 12.70, 3.66, 3.25, and 2.04%, respectively. As can be observed, the average absolute values of the relative error for naphtha, distillate, and residue are lower than 5%.

3.3. Numerical Solution of Model Equations. The properties of the trickle-bed reactor and operational conditions and the fluid properties are presented in Table 2. In this table, the properties of the VGO feed and hydrocracking products were analyzed based on the ASTM standard procedures. Moreover, the kinetic parameters of the model (i.e., \( k_1 - k_8 \)) and specifications of the reactor were the reported values in the previous research. A two-dimensional model was assembled to simulate the hydrocracking of the VGO utilizing the CFD method based on a finite-element scheme. The solver (PARDISO) version 5.3 of COMSOL package was applied as a linear solver in the simulations. A system with the characteristics of RAM 4.00 GB (2.98 GB applicable) and Intel CoreTM i5 CPU M 480@2.67 GHz and 64-bit operating system was applied to analyze the equations.
which is reasonably accurate to investigate the mass transfer in the reactor using the developed model. Sadighi\textsuperscript{30} developed a five-lump model using axial-dispersion lumped kinetics for the VGO hydrocracking, and the average absolute deviation (AAD %) was found to be 10.4%, which shows that the current model is effective and useful with less error.

The average absolute deviation (AAD%) and the mean square error (MSE%) were used to verify the validity and usability of the developed model. AAD% and MSE% can be determined using the following equations

\[
\text{AAD\%} = \frac{\sum_{n=1}^{N_f} \sum_{i=F}^{G} (Y_{n}^{\text{exp}} - Y_{n}^{\text{model}})^2}{N_f} \times 100 \tag{15}
\]

\[
\text{MSE\%} = \frac{\sum_{n=1}^{N_f} \sum_{i=F}^{G} (Y_{n}^{\text{exp}} - Y_{n}^{\text{model}})^2}{N_f} \times 10000 \tag{16}
\]

Table 3 provides the AAD% and MSE% of our previous study\textsuperscript{19} and the currently developed model. It was observed that the AAD% and MSE% of gas, naphtha distillate, and residue were decreased in the current study. It means that the currently developed model is more reliable and accurate to predict the yield of the feed and products.

4.2. Concentration Distribution of Feed and Products. Figure 4 shows the surface concentration distribution of distillate, feed, naphtha, and gas along the length of the reactor. As shown in Figure 4, initially the feed flows from the bottom of the reactor at \( z = 0 \), where the concentration of the feed is the highest, while its minimum value is at the outlet (\( z = L \)). As the feed flows through the packed-bed reactor, the feed was

![Figure 4. Surface concentration distribution of feed (a), distillate (b), naphtha (c), and gas (d) in the length of the reactor.](image)

![Figure 5. Influence of feed velocity on the VGO concentration alongside the reactor.](image)
converted to the products. Conversely, the highest concentration of the products is in the reactor outlet ($z = L$). The mass transfer mechanisms in the reactor are diffusion and convection. In the axial direction, the dominant mechanism is the convection mass transfer because the feed flows in the $z$-direction inside the reactor. The diffusion mechanism plays a momentous role in the $r$-direction due to huge concentration differences in the radial direction.

The concentration of feed alongside the length of the reactor for various values of feed flow rates is depicted in Figure 5. The increase in the feed flow rate increases the feed concentration in the outlet of the reactor. The residue concentration at the outlet of the reactor improved from 420 to 500 kg·m$^{-3}$, with the enhancement of feed flow rate from 0.1568 to 0.2059 kg·h$^{-1}$ which means that the lower amount of the feed was converted to the products. It can be attributed to the fact that increasing the feed flow rate decreases the residence time of feed in the reactor, which, in turn, decreases the feed converted to the products.

The products including distilled, naphtha, and gas concentrations along the reactor in terms of the feed mass flow rate is illustrated in Figure 6. As seen, there is a linear increase in the concentration of naphtha along the reactor. However, the change in distillate and gas concentrations in the bottom half of the reactor is a bit higher than that in the top half of the reactor. The enhancement of the feed flow rate from 0.1568 to 0.2059 kg·h$^{-1}$ resulted in a decrease of the outlet distillate (245–207 kg·m$^{-3}$), naphtha (180–84 kg·m$^{-3}$), and gas (26–21 kg·m$^{-3}$) concentrations.

5. CONCLUSIONS

A pilot-scale hydrocracking reactor was modeled in this investigation considering the mass and momentum transfer, continuous kinetic lumping technique, and physical properties of components. The computational fluid dynamic simulation of the reactor allows tracking the reaction dynamics to predict the concentration profiles and its alterations along the reactor at different operating conditions. The average absolute value of the relative error for prediction of the yield of gas, naphtha, distillate, and residue using the proposed model was obtained 12.70, 3.66, 3.25, and 2.04%, respectively. The evaluation of the results showed that the developed model and CFD method are more accurate than the previous model for the reactor. Generally, it can be concluded that based on the modeling results, which the current CFD model explains better, the hydrocracking of the VGO occurs in the studied reaction conditions.

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Figure 6. Impact of feed velocity on the product concentration alongside the reactor.
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Notes
The authors declare no competing financial interest.

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