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MODELING A VACUUM GAS OIL HYDROCRACKING REACTOR USING AXIAL-DISPERSION LUMPED KINETICS

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Abstract

Hydrocracking of vacuum gas oil (VGO) is used in refinery to produce precious products such as diesel, kerosene and naphtha. In this research, a pilot scale reactor has been used to study the hydrocracking behavior of VGO under the conditions recommended by the catalyst vendor and literature in terms lumping of feed and products. A five lumped kinetic model including thirteen parameters is proposed to predict the yield of the products. The lumping scheme is based on the most added values, i.e. gas, naphtha, kerosene, diesel and the unconverted VGO. At first, the hydrocracking reactor was modeled as an ideal plug flow and its kinetic parameters were estimated by a weighted least square function. The average absolute deviation (*AAD%*) of the yield prediction by using this strategy is 11.86%, 2.66% lower than the conventional ones. Then, a better agreement between the model outputs and the experimental information, with the *AAD%* of 10.4% is obtained when selective axial-dispersion coefficients were entered in the model.

Keywords: Hydrocracking; Vacuum Gas Oil; Lump kinetic model; Non-ideal flow; Axial-dispersion

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1. Introduction

Of every barrel of crude oil currently refined worldwide, over 45 percent on average historically receives some hydroprocessing process, which is divided into three categories: hydrocracking, hydrorefining and hydrotreating [1]. This percentage continues to grow and varies with the geographical area. Hydrocracking is one of the most interested upgrading processes, widely spread to convert low precious vacuum gas oil to required and valuable transportation fuels such as diesel and gasoline [2]. In order to have an effective design and a perfect control over it, a model is needed to predict product yields and qualities versus variables such as space velocity and temperature. Moreover, the model can also be used to select the suitable hydro-cracking catalysts [3]. However, the complexity of hydrocracking feed makes it extremely difficult to characterize and describe its kinetic at a molecular level [4]. One approach to simplify the problem is to consider the partition of the components into a few equivalent classes called lumps or lumping technique, and then assume each class as an independent entity [5]. Developing simple kinetic models (e.g., power-law model) for complex catalytic reactions is a common approach that can give basic information for catalyst screening, reactor design and optimization [6,7].

This kind of modeling is proposed by several researches in which hydrocracking process was modeled with three-lump [8-11], four-lump [3,12], five-lump [13-16], six-lump [17,18], seven-lump[19] and eight-lump [20] approaches. All of these articles have one approach in common that was the reactor as an ideal plug flow, which was hardly achievable in pilot scale reactors [21, 22].

In a different approach, the description of the hydrocracking kinetic of Kuwait VGO feed was done according to TBP distribution curve and axial description kinetic model [23]. The same approach and resulted parameters were used later to describe the behavior of the concentration of heavy petroleum fraction constituents during the hydrocracking process (paraffins, naphthenes and aromatics) [24].

The present study has focused on developing a network, according to a five-lump approach to predict the most added value products including gas (lights and LPG), naphtha, kerosene and diesel in a pilot scale hydrocracking reactor, which its feed is heavy Iranian VGO. The advantages of this work are: I) by separating kerosene and diesel, the evaluation of the catalyst can be done better because each of these desired products has different worth, usage and finishing process II) by using a weighted least square expression for estimating the kinetic parameters, the average absolute deviation (AAD) of the model is decreased III) for the reason of indispensable non-idealities, an axial-dispersion kinetic model is applied to increase the accuracy of the model in comparison to an ideal flow assumption. The nobility of this work is to consider selective axial-dispersion coefficients in the model, integrated to lumped components, to predict the product yields of a hydrocracking reactor more accurately.

2. Hydrocracking kinetic model

In this investigation, the feed and the product are lumped into VGO, diesel, kerosene, naphtha and gas to predict all valuable products of a pilot plant reactor. Fig. 1 depicts the reaction pathways associated with the strategy. Note that if all reaction pathways are considered, the model including twenty kinetic parameters, ten frequency factors and ten apparent activation energies that should be estimated by using experimental data and it is too laborious. Some judgments are normally welcomed to reduce the model complexity, without scarifying the accuracy. Upon close scrutiny of the system, the model can be reduced, requiring less kinetic parameters. It can be done according to the magnitude analysis at the average operating temperature.

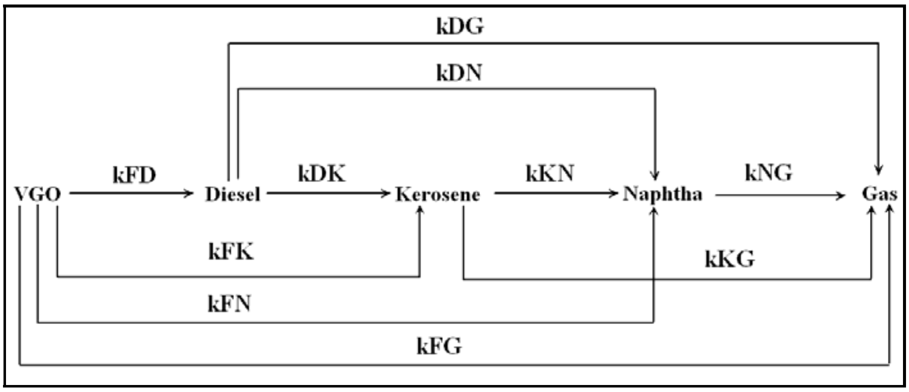

Figure 1. The complete 5-lump kinetic model

3. Experimental

3.1 Device

The experiment was conducted in the pilot system (‘Geomechanique BL-2’). This plant that belongs to the catalysis research center (CRC) of research institute of petroleum industry (RIPI), and it can tolerate temperature and pressure up to 500°C and 300 bar, respectively. All experiments were supported and conducted by CRC [25]. The physical properties of the feed and product samples were determined according to the ASTM standard procedures.

3.2 Feed and the Catalyst

Hydrocracking was carried out using fresh vacuum gas oil (VGO), taken directly from the vacuum tower of a 100,000 BPD refinery. Its physical properties are shown in Table 1. To do the experiments, the reactor was charged with a commercial amorphous bifunctional catalyst, which its characterization is presented in Table 2. The quantity of loaded catalyst was about 33 g (50 cm^3).

3.3 Test conditions

Hycrocracking was carried out under the following operating conditions: **1.** H_2/HC=1780 Nm^3/Sm^3; **2.** LHSV=0.5, 1, 1.2, 1.5 and 2 hr^{-1}; **3.** temperature=380°C and 400°C, and **4.**

pressure =156 bar. The operating pressure and H_2/HC have been recommended by the catalyst vendor. The range of LHSV for this catalyst was normally between 1 and 1.2 hr^{-1}. However, it is preferably 1 hr^{-1}. Although the recommended range for LHSV in the literature for this process is between 1 and 1.5 hr^{-1} [26].

Table 1. Properties of fresh vacuum gas oil

Sp.gr at 15°C	-	0.908
Sulfur	wt%	1.73
Total Nitrogen	wt%	0.09
Aromatics	wt%	27.3
Distillation vol% (D1160)		
IBP	° C	332
10%	° C	402
30%	° C	427
50%	° C	447
70%	° C	464
90%	° C	490
FBP	° C	515

Table 2. Catalyst specifications of hydrocracking process

Shape	-	Spherical
Mesh	-	10-20
Bulk Density	kg/m3	654
Density(solid)	kg/m3	2500
Surface Area	m2/g	270
App. porosity	cm3/g	1.13
	Components	
Base	Silica Alumina	
SiO_2	wt %	55.39
Al_2O_3	wt %	9.27
WO_3	wt %	24.53
NiO	wt %	3.55
Cao	wt %	0.46
Fe_2O_3	wt %	Trace

4. Modeling approach

Mathematical models for the VGO hydrocracking process, in a trickle-bed regime, can be complex due to many microscopic and macroscopic effects occurring inside the reactor, such as flow pattern of phases, size and shape of the catalyst, wetting the catalyst pores with liquid phase, pressure drop, thermal effects and the catalyst surface reaction [27]. Therefore, it is more practical to reduce the complexity of the reactor, focusing only on momentous process variables. This approach suggests the development of simpler models, incorporating fewest possible parameters. In this work, the following assumptions have been made to simplify the model:

1- Hydrocracking is a first order hydrocracking reaction [28]. Since hydrogen is present in excess, the rate of hydrocracking can be supposed to be independent of the hydrogen concentration. Therefore, the rate of reaction does not depend explicitly on partial pressure of hydrogen.
2- The pilot reactor operated under isothermal conditions.
3- Selective axial-dispersion coefficients were applied. So there was a different diffusion rate for each lump.
4- Hydrogen feed was pure.
5- The feed and all products are in the liquid phase
6- The operation of the pilot unit was steady state
7- Catalyst activity did not change with time. Hence simulation was only valid for the start of run.

4.1 Kinetic model

For each lump, the reaction rate (R) is the function of mass concentration (C) and kinetic parameters (k_0 and E). Based on mentioned assumptions, the kinetic constants of the model can be expressed as

Vacuum gas oil or Feed (F): $$k_{Fj} = k_{0Fj} \exp(\frac{-E_{Fj}}{RT}) \qquad (1)$$

where j represents diesel (D), kerosene (K), naphtha (N) and gas (G).

Diesel (D): $$k_{Dj'} = k_{0Dj'} \exp(\frac{-E_{Dj'}}{RT}) \qquad (2)$$

where j' represents kerosene (K), naphtha (N) and gas (G).

Kerosene (K): $$k_{Kj''} = k_{0Kj''} \exp(\frac{-E_{Kj''}}{RT}) \quad (3)$$

where j'' represents naphtha (N) and gas (G).

Naphtha (N): $$k_{NG} = k_{0NG} \exp(\frac{-E_{NG}}{RT}) \quad (4)$$

Here, T and R are bed temperature (K) and gas law constant (kcal mol^{-1} K^{-1}), respectively. The reaction rates (R) can be defined as the following.

Vacuum gas oil reaction (R_F): $$R_F = \sum_{j=D}^{G} k_{Fj} C_F \quad (5)$$

Diesel (R_D): $$R_D = k_{FD} C_F - \sum_{j'=K}^{G} k_{Dj'} C_D \quad (6)$$

Kerosene (R_K): $$R_K = k_{FK} C_F + k_{DK} C_D - \sum_{j''=N}^{G} k_{Kj''} C_K \quad (7)$$

Naphtha (R_N): $$R_N = k_{FN} C_F + k_{DN} C_D + k_{KN} C_K - k_{NG} C_N \quad (8)$$

Gas (R_G): $$R_G = k_{FG} C_F + k_{DG} C_D + k_{KG} C_K + k_{NG} C_N \quad (9)$$

4.2 Mass balance equations

The overall mass balance for all lumps is

$$\frac{\partial (C_j U)}{\partial Z} - D_j \frac{\partial^2 C_j}{\partial Z^2} \pm \eta.\varepsilon.R_j = 0 \quad (10)$$

Here the "+" sign is for reactant (feed or VGO) and the "–" sign is for the products. Subscript j represents feed (F), diesel (D), kerosene (K), naphtha (N) and gas (G).

The mass balance equations are solved numerically by using the following boundary conditions [29]:

$$U(C_j^{\infty} - C_j) = D_j \frac{dC_j}{dZ} \quad \text{at} \quad Z = 0 \quad (11)$$

And

$$\frac{dC_j}{dZ} = 0 \quad \text{at} \quad Z = L \quad (12)$$

Here U is the intrinsic velocity of the stream through the reactor; C_j^{∞} is the initial mass concentration; C_j is the product mass concentration; D is the axial-dispersion coefficient; Z is the axial position; η is the catalyst effectiveness factor, and ε is the bed void fraction.

The effectiveness factor for a spherical catalyst in trickle bed regime is considered to be 0.8 [30]. Also the bed void fraction for the catalyst bed is 0.264. The intrinsic velocity and yield of products are

$$U = \frac{\upsilon}{A.\varepsilon} \quad (13)$$

$$Y_j = \frac{C_j.\nu}{F} \quad (14)$$

$$\upsilon = \frac{F}{\rho} \quad (15)$$

$$F = \sum_{j=F}^{G} C_j \upsilon \tag{16}$$

Here Y , υ , F and A are yield of the product, volume flow rate along the axial direction, mass flow rate and cross section of the reactor, respectively. The only unknown variable is the density of stream through the reactor, ρ , which can be expressed as follows:

$$\frac{1}{\rho_0} = \sum_{i=F}^{G} \frac{Y_j}{\rho_j} \tag{17}$$

where ρ_j is the density of each lump (Table 3). It should be noted that the density evaluated by Eq. (17) (ρ_0) is standard density, which can be used to determine density at the reactor condition (ρ) by the Standing-Katz correlation [31]. In deviating from the SI system we give the Eq. (18) with the original units:

$$\rho(p,T) = \rho_0 + \Delta\rho_p - \Delta\rho_T \tag{18}$$

where ρ_0 represents the density at standard conditions in lb/ft^3.

The pressure dependence can be evaluated by:

$$\begin{aligned}\Delta\rho_p &= [0.167 + 16.181 \times 10^{-0.0425.\rho_0}].[\frac{p}{1000}] - \\ &0.01 \times [0.299 + 263 \times 10^{-0.0603.\rho_0}].[\frac{p}{1000}]^2\end{aligned} \tag{19}$$

where p is the pressure in Pisa. Since the density drops by increasing temperature, a correction with the temperature in ^{0}R is needed:

$$\begin{aligned}\Delta\rho_T(i) &= [0.0133 + 152.4 \times (\rho_0 + \Delta\rho_p)^{-2.45}].[T - 520] - \\ &[8.1 \times 10^{-6} - 0.0622 \times 10^{-0.764.(\rho_0 + \Delta\rho_p)}].[T - 520]^2\end{aligned} \tag{20}$$

Table 3. Average properties of hydrocracking product

	Sp.gr @15.5 °C	IBP-FBP (°C)
Gas	0.35	40$^-$
Naphtha	0.744	40-141
Kerosene	0.796	141-260
Diesel	0.823	260-370
Residue	0.908	370$^+$

4.3 Numerical solution

To predict the product yield, all equations should be solved simultaneously. To do this, at first Eq. (10) is converted into a set of algebraic equations by applying the following backward and central difference expressions

$$\frac{\partial(C_j U)}{\partial Z} = \frac{(C_j U)_i - (C_j U)_{i-1}}{h} \tag{21}$$

$$\frac{\partial^2 C_j}{\partial Z^2} = \frac{C_j(i+1) - 2C_j(i) + C_j(i-1)}{h^2} \tag{22}$$

where the subscript i and the variable h denote step number and step lengths, respectively. The number of steps is 200 for the hydrocracking reactor, which is recommended in the literature for trickle bed reactors [32]. All produced algebraic equations are solved by using Aspen Custom Modeler program (ACM ver. 11.1, AspenTech 2001).

4.4 Parameter estimation

For the parameter estimation two methods have been used as follows.

4.4.1 Unweighted method

In this method, the sum of squared error, SQE_1, as given below, is minimized whilst all weight function (w_j) are one.

$$SQE_1 = \sum_{k=1}^{N_t} \sum_{j=F}^{G} w_j .(Y_{kj}{}^{meas} - Y_{kj}{}^{pred})^2 \tag{23}$$

where N_t, $Y_{kj}{}^{meas}$ and $Y_{kj}{}^{pred}$ are the numbers of test runs, measured yield and the predicted one, respectively.

4.4.2 Weighted method

Before minimizing Eq. (23), the weight functions (w) are determined by minimizing the following expression [33].

$$SQE_2 = \sum_{k=1}^{N_t} \sum_{j=F}^{G} (w_j Y_{kj}{}^{meas} - w_{ref} Y_{k\,ref})^2 \tag{24}$$

where w_j in Eq. (24) is the weight coefficient of lumps, which plays a crucial role to have an evenly distributed $AAD\%$ along the predicted yield for the lump with higher yield like diesel and the lump with lower yield like naphtha. The subscript ref in Eq. (24) refers to the lump with the lowest yield. Hence, it is expected to have a more accurate model, discussed later.

At first, in order to estimate weight parameters, the objective function presented in Eq. (24) is minimized by the solver tool in Excel package, using Newton search method. Then Eq. (23) is minimized by using these weights and sequencing NL2Sol and Nelder-mead algorithm, which are available in Aspen Custom Modeler software. NL2Sol algorithm is a variation on Newton's method in which part of the Hessian matrix is computed exactly and part is approximated by a secant (quasi-Newton) updating method.

To investigate the suitability of the fitting, the average absolute deviation of predictions (*AAD%*), presented in the literature [34], was calculated by using Eq. (25).

$$AAD\% = 100 \frac{\sum_{k=1}^{N_t} \sqrt{\dfrac{(Y_k{}^{meas} - Y_k{}^{pred})^2}{Y_k{}^{meas\,2}}}}{N_t} \% \tag{25}$$

5. Results and discussion

5.1 Lump characteristics

The main products of the process were: gases (dry light gases and LPG), naphtha, kerosene, diesel and VGO. The average density and boiling point range of these products are presented in Table 3. Based on the analyzed data, it is found that the distillation property of the residue or unconverted oil is close to that of fresh VGO, so the consideration of them as one lump is not an irrational assumption.

5.2 Modeling results

At first, it was assumed that the flow regime of the reactor was an ideal plug one, i.e. all axial-dispersion coefficients in Eq. (10) were considered to be zero. The estimated twenty kinetic parameters using unweighted method are detailed in Table 4. The rate constants for all reactions were also calculated in the average operating temperature (390^{0}C). To compare the simulated yields with the measured values, the average $AAD\%$ of lumps was calculated and it is presented in Table 5 under the name of complete-unweighted model.

It is observed that rate constants for conversion of feed to middle distillates (k_{FD} and k_{FK}) are higher than those of feed to naphtha. Furthermore, the rate constant for cracking naphtha to gas (k_{NG}) is tremendously high, which seems to be reasonable because of the simplicity of cracking light chains of naphtha in comparison to heavier and more stable chains of diesel and kerosene. It means that middle distillates play a minor role in producing gas in hydrocracking process. These phenomena can justify the lowest yield for naphtha by an amorphous hydrocracking catalyst [35, 36].

Table 4. Kinetic parameters for the complete-unweighted network

Frequency Factor ($m^3.hr^{-1}.kg\ cat^{-1}$)		Activation Energy (kcal/mol)		Rate Constant ($kg.hr^{-1}.kg\ cat^{-1}$)	
k_{0FD}	2.57E+08	E_{FD}	23.52	k_{FD}	4.53
k_{0Fk}	1.64E+16	E_{Fk}	50.37	k_{Fk}	0.40
k_{0FN}	5.82E+08	E_{FN}	41.61	k_{FN}	1.11E-05
k_{0FG}	51.91	E_{FG}	5.44	k_{FG}	0.836
k_{0DK}	2.10E+15	E_{DK}	44.72	k_{Dk}	3.773
k_{0DN}	2.00E+15	E_{DN}	46.16	k_{DN}	1.20
k_{0DG}	4.70	E_{DG}	42.66	k_{DG}	4.03E-14
k_{0KN}	3.146E+07	E_{KN}	21.03	k_{KN}	3.66
k_{0KG}	0.01	E_{KG}	0.10	k_{KG}	4.65E-03
k_{0NG}	11.87	E_{NG}	0	k_{NG}	11.86

Table 5. The $AAD\%$ for the different strategies in the plug flow reactor

Lump	Complete-unweighted model	Complete-weighted model	Reduced-weighted model	Axial-dispersion model
Gas	5.29	7.05	6.65	7.79
Naphtha	25.41	14.94	15.94	12.38
Kerosene	19.04	17.99	17.20	15.14
Diesel	14.09	15.04	11.13	10.58
Un.VGO	8.75	9.42	8.39	6.11
Ave.	14.52	12.88	11.86	10.4

The next try for parameter estimation is done by using the factors presented in Table 6, which were estimated from minimizing the Eq. (24). The resulted kinetic parameters are detailed in Table 7. After applying these kinetic parameters, the average $AAD\%$ of the predicted hydrocracking yields is decreased to 12.88%, detailed in Table 5 under the name of complete-weighted model. It is confirmed that the introduced weighted method is more efficient to estimate the kinetic parameters, which are involved in the hydrocracking model.

Table 7 shows that three paths including feed to naphtha, diesel to gas and kerosene to gas can be ignorable due to low constant rates. In addition, the activation energy for converting naphtha to gas is zero. In order to reduce the number of kinetic parameters involved in the model, those with lower rate constants can be omitted during parameter estimation. Now, thirteen remained parameters should be estimated by fifty observations, creating more acceptable degree of freedom. After eliminating the least possible reactions, the reduced reaction network is depicted in Fig. 2.

Table 6. Estimated factors for weighted estimation

Lump	Weight factor
Gas	0.593
Naphtha	1.51
Kerosene	0.549
Diesel	0.243
Unconverted	0.138

Table 7. Kinetic parameters for the complete-weighted network

Frequency Factor ($m^3.hr^{-1}.m^3\ cat^{-1}$)		Activation Energy (kcal/mol)		Rate constant ($m^3.hr^{-1}.m^3\ cat^{-1}$)	
k_{0FD}	2.25E+08	E_{FD}	23.51	k_{FD}	4
k_{0Fk}	2.34E+16	E_{Fk}	49.63	k_{Fk}	1.01
k_{0FN}	9.30E+08	E_{FN}	41.34	k_{FN}	2.18E-5
k_{0FG}	52.84	E_{FG}	5.61	k_{FG}	0.745
k_{0DK}	7.95E+14	E_{DK}	45.39	k_{Dk}	0.862
k_{0DN}	3.00E+15	E_{DN}	45.72	k_{DN}	2.53
k_{0DG}	5.22	E_{DG}	87.38	k_{DG}	8.04E-29
k_{0KN}	1.080E+07	E_{KN}	22.13	k_{KN}	0.54
k_{0KG}	0.00	E_{KG}	0.13	k_{KG}	2.08E-03
k_{0NG}	12.43	E_{NG}	0	k_{NG}	12.43

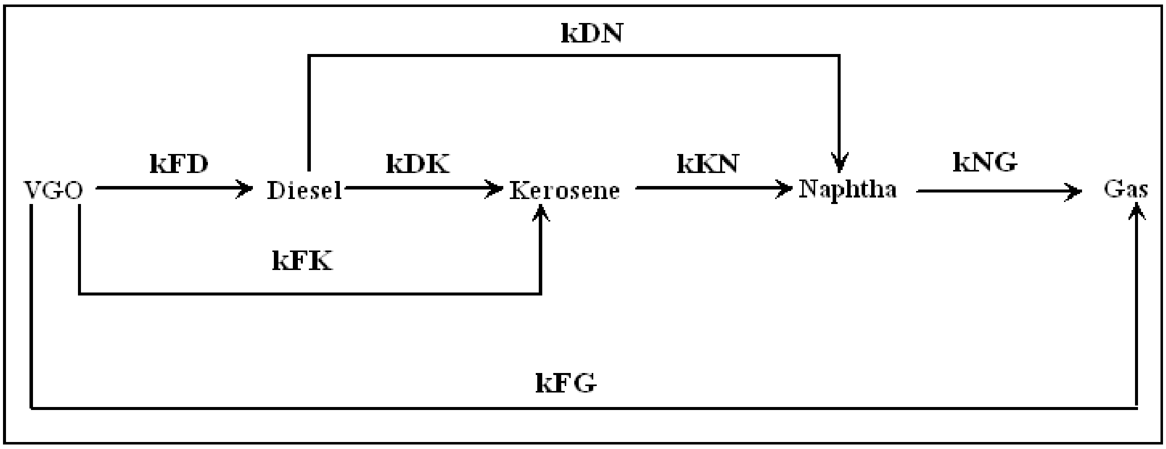

Figure 2. The reduced 5-lump kinetic network

The kinetic parameters of the reduced model were estimated again using measured data, producing new values, which are detailed in Table 8. Upon comparing the measured data with the model predictions, the average $AAD\%$ for the reduced model is reached to 11.86%, flagrantly improved in comparison to the complete network, similar to the previous work for thermal cracking of vacuum residue that claimed prediction using reduced model is more accurate [37]. The average $AAD\%$ of lumps resulted by this approach is presented in Table 5 under the name of reduced-weighted model.

The next try at parameter estimation was done by assuming the existence of axial-dispersion, affecting the ideal plug flow of reactor, which can be simulated by non-zero axial-dispersion coefficients for lumps in Eq. (10). Now, to estimate required parameters, Eq. (23) is minimized by manipulating axial-dispersion coefficients whilst the kinetic parameters are those presented in Table 8. It means that the deviation from the ideal plug flow regime is modeled by applying axial-dispersion coefficients.

During estimation, it was found that the axial-dispersion coefficients between 380^{0}C and 400^{0}C were different. Since diffusion factors are dependent on temperature, this discrepancy is explicable.

In Table 9, the $AAD\%$ of the predicted yields at 380^{0}C in all operating LHSVs are tabulated. In this Table, the $AAD\%$ of the reduced model, showing the most accuracy in the ideal plug flow, is compared with the prediction of the axial-dispersion model. From Table 9, It is observed that for the LHSV=0.5 hr^{-1} with the temperature of 380^{0}C, the yield prediction is considerably improved, showing high axial-dispersion phenomenon in this condition due to the low intrinsic velocity. Also, for the LHSV=2 hr^{-1}, increasing the accuracy is not considerable, which confirms deviation from the ideal plug flow in this operating condition is not strongly dependent on axial-dispersion phenomenon. For the LHSV ranging from 1 to 1.5 hr^{-1}, axial- dispersion not only does not improve the accuracy but also increases the deviation. It can be concluded that the flow in this region is close to ideal plug so it is an appropriate flow regime to perform hydrocracking process.

Table 8. Kinetic parameters for the reduced-weighted network

Frequency Factor (m^3.hr^{-1}.m^3 cat^{-1})		Activation Energy (kcal/mol)		Rate constant (m^3.hr^{-1}.m^3 cat^{-1})	
k_{0FD}	9.67E+05	E_{FD}	16.36	k_{FD}	4
k_{0Fk}	7.79E+16	E_{Fk}	51.09	k_{Fk}	1.11
k_{0FN}	-	E_{FN}	-	k_{FN}	-
k_{0FG}	62.35	E_{FG}	5.82	k_{FG}	0.753
k_{0DK}	2.48E+16	E_{DK}	51.43	k_{Dk}	0.273
k_{0DN}	3.61E+15	E_{DN}	45.83	k_{DN}	2.79
k_{0DG}	-	E_{DG}	-	k_{DG}	-
k_{0KN}	1.024E+01	E_{KN}	7.18	k_{KN}	0.04
k_{0KG}	-	E_{KG}	-	k_{KG}	-
k_{0NG}	11.93	E_{NG}	-	k_{NG}	11.93

Table 9. ADD% for the reduced-weighted plug flow and the axial-dispersion models at 380^{0}C

LHSV(hr^{-1})	Reduced weighted model	Axial-dispersion model
0.5	27.88	11.38
1	3.08	3.49
1.2	13.7	14. 3
1.5	16.71	17.59
2	26.93	26.28

In Table 10 the estimated axial-dispersion coefficients for the LHSV ranging from 0.5 to 2 hr^{-1} with the temperature of 380^{0}C is tabulated. It is observed that they decrease in order as lighter lump (naphtha) to heavier lump (VGO), consistent with this phenomenon that lighter components have higher molecular diffusion.

Table 10. Axial-dispersion coefficients for the hydrocracking lumps at 380^{0}C

Lump	D_j @ 380^{0}C
Gas	0
Naphtha	1.04E-03
Kerosene	7.35E-04
Diesel	4.299E-04
Un. VGO	3.831E-04

Table 11. ADD% for the Reduced weighted plug flow and the axial-dispersion models at 400^{0}C

LHSV(hr^{-1})	Reduced-weighted model	Axial-dispersion model
0.5	4.19	4.19
1	7.25	7.25
1.2	4.94	4.94
1.5	6.55	6.55
2	8.02	8.02

In Table 11, the $AAD\%$ of the predicted yields at 400^{0}C in all operating LHSVs, comparing with the reduced model, are tabulated. It is observed that the $AAD\%$ of axial- dispersion model is the same as reduced model because of negligible axial-dispersion effects at this temperature. Moreover, for the LHSV=0.5 hr^{-1} and LHSV=2 hr^{-1} at 400^{0}C, the predictions are markedly more accurate than the same LHSVs at 380^{0}C. This is due to the higher heat and mass diffusion as well as higher intrinsic velocity at 400^{0}C, creating lower non-idealities and mass resistances through the catalyst bed.

The predicted data tabulated in Table 9 and Table 11 reveal that the reduced model calculated yields for LHSV ranging from 1 to 1.5 hr^{-1} at 380 and 400^{0}C temperatures are reasonably fit the experimental data for the five lumps with the average $AAD\%$ of 8.705%. Therefore, it can be concluded that for the pilot scale VGO hydrocracking reactor, assuming the flow of reactor as an ideal plug one is not far from the reality, especially at the high temperatures.

The parity diagrams of the products obtained in the hydrocracking of VGO are shown in Fig. 3 through Fig. 7, confirming reasonably agreement between experimental data and predicted yields by the model. Hence, the axial-dispersion kinetic model can acceptably simulate the behavior of the understudy hydrocracking reactor. Furthermore, from Figs. 4 and 5 it can be understood that there is an acceptable agreement between the experimental and predicted values for naphtha and kerosene lumps. However, the high absolute deviation of these lumps, reported in Table 5, is due to their low yields when they are dominators in Eq. (25). This reason can be interpreted the same for the diesel (Fig. 6). Although it has low average absolute deviation, its parity diagram shows less fit.

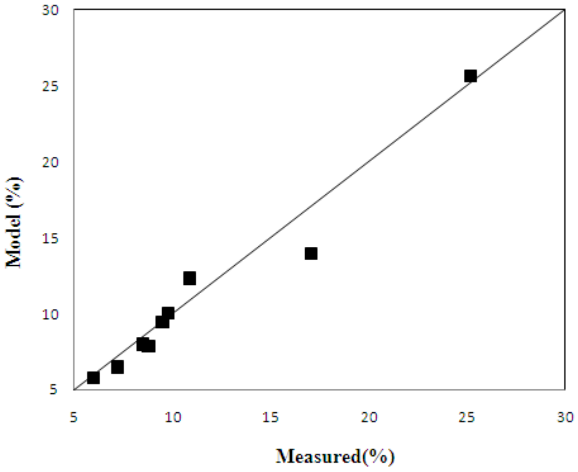

Figure 3. Parity plot for gas resulted by axial-dispersion model

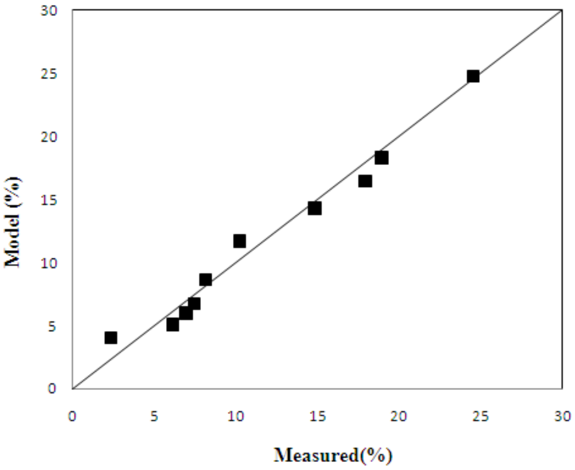

Figure 4. Parity plot for naphtha resulted by axial-dispersion model

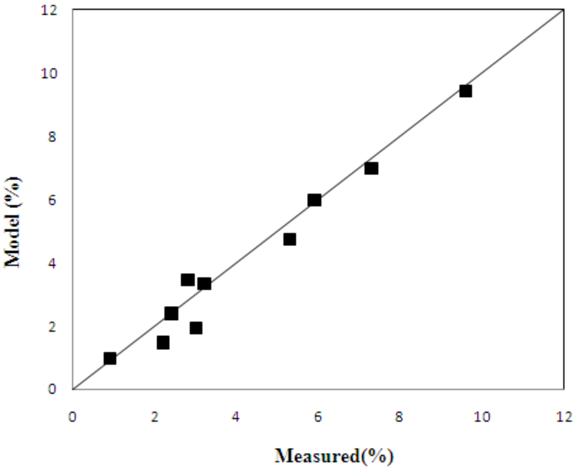

Figure 5. Parity plot for kerosene resulted by axial-dispersion model

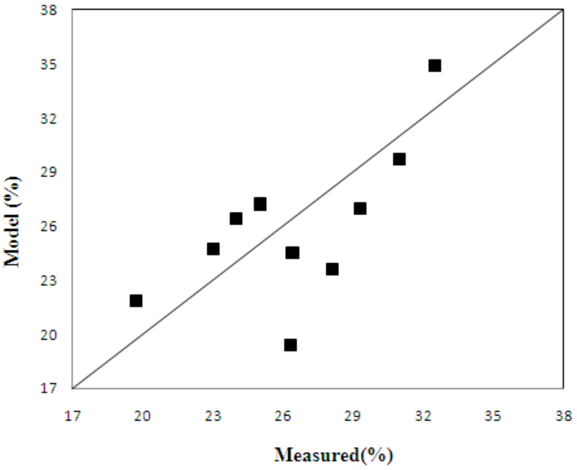

Figure 6. Parity plot for diesel resulted by axial-dispersion model

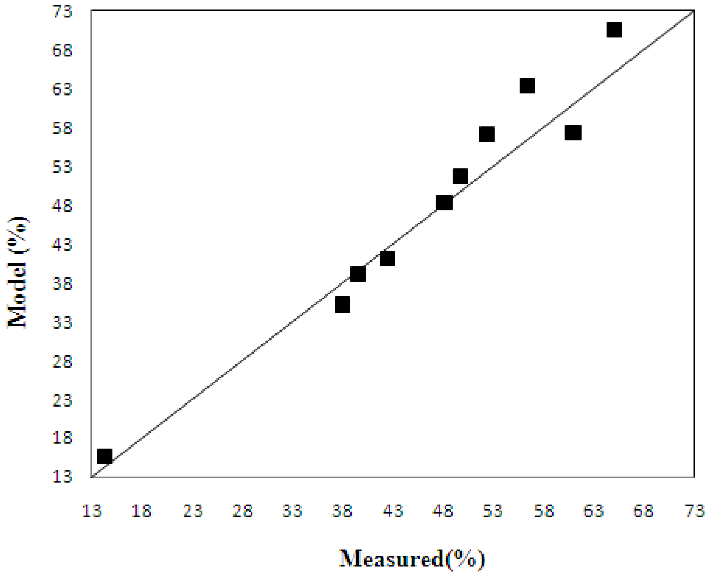

Figure 7. Parity plot for unconverted VGO resulted by axial-dispersion model

6. Conclusions

A five lump model is developed for the hydrocracking of vacuum gas oil feedstock. The lumps are selected on the basis of the valuable products in a commercial refinery. Rate analysis is used to identify the least possible reaction pathways. From this analysis, it is concluded that the hydrocracking of VGO in an ideal plug flow reactor can be described by a reduced kinetic network including seven reaction pathways and thirteen kinetic parameters. The kinetic parameters of this network, estimated by an introduced weighted least square expression, predicts the yield of the VGO hydrocracking products more accurate than those estimated using conventional methods. The proposed approach can decrease the average $AAD\%$ of prediction from 14.52% to 11.86%.

Because of some non-idealities, which are indispensable in a trickle bed pilot scale reactor, modeling the hydrocracking process by considering the axial-dispersion through the catalyst bed can be more efficient. The developed model, which includes four axial-dispersion coefficients, can predict the yield of products with the average $AAD\%$ of 10.4%.

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