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SIMULATION AND MODELING OF HYDRO CRACKING REACTR TO REDUCE POLLUTION CAUSED BY REFINERIES

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ABSTRACT

Hydro cracking of heavy oil is used in refinery to produce invaluable products. In this research, a model of hydro cracking reactor has been used to study the behavior of heavy oil in hydro cracking under the conditions recommended by literature in terms lumping of feed and products. The lumping scheme is based on five lumps include: heavy oil, vacuum oil, distillates, naphtha and gases. The first order kinetics was assumed for the conversion in the model and the system is modeled as an isothermal tubular reactor. MATLAB 6.1 was used to solve the model for a five lump scheme for different values of feed velocity, and temperature.

Keywords: Hydro cracking, heavy oil, modeling, reduce pollution, refineries.

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محاكاة ونمذجة مفاعل التكسير الهيدروجيني للحد من التلوث الناجم عن المصافي

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الخلاصة

يستعمل التكسير الهيدروجيني للنفط الثقيل في المصافي لانتاج منتجات ذات قيمة، وفي هذا البحث تم استخدام موديل لمفاعل التكسير الهيدروجيني لدراسة سلوك النفط الثقيل بالتكسير الهيدروجيني تحت الظروف التي توصي بها الادبيات العلمية بأخذ مقطع للناتج والللقيم الداخلة والموديل للمقطع يستند الى خمس مقاطع تتضمن: النفط الثقيل ونفط فراغي والقطارات والنفثا والغازات، وتم افتراض نموذج حركية من الدرجة الاولى للتحول وتم نمذجة مفاعل انبوبي ثابت حرارياً، وأستخدم برنامج ما تلاب 6.1 لحل الموديل ذو الخمس مقاطع لقيم مختلفة من سرعة القيم، ودرجة الحرارة.

الكلمات المفتاحية: التكسير الهيدروجيني، النفط الثقيل، نمذجة، الحد من التلوث، المصافي.

INTRODUCTION

Hydro cracking is commonly used to process feed stocks that are unsuitable for catalytic cracking or reforming, due to high concentrations of either polycyclic aromatics, or sulfur, or nitrogen compounds, which act as catalyst poisons. The primary function of hydrogen is to prevent the formation of polycyclic aromatics compounds reduce tar formation and to convert sulfur and nitrogen compounds presented in the feed stocks to hydrogen sulfide and ammonia **(Bhutani 2007)**. Furthermore, the vast versatility of hydro cracking makes possible to counterpoise product supply according to coveting. Oil fractions are (hydro) processed in the refinery primarily to fabrication conveyor fuels that immanent for our community **(Sadighi *et al.,* 2012)**. Exemplary for industrial processes, optimum operation is exactingly to assuring gainfully, and like this assignment entails use of process models. These models are used to anticipating the product yields and qualities, and are beneficial for sensitivity analysis, consequently effectuating of operating parameters such as reactor temperature, pressure, space velocity, as well as others on product yields and qualities, it could be comprehended. The models can also be used for process optimization and control, design of new units and selection of appropriate hydro cracking catalysts **(Valavarasu *et al.,* 2005)**. According to the obvious nature of feedstock for hydro cracking units which is considered vastly complex and the hard disposable liquids that be conversely to the more pure units which take this treatment liquids to other useful chemical industry destinations **(Becker *et al.,* 2016)**. In general at hydro cracking process extra amount of hydrogen will be available to saturate fractions of feedstock that admittedly consider as a high boiling point as feed; thereupon that hydrogen lets to get middle distillates assuredly low boiling point products **(Ignacio *et al.,* 2010)**. The main products that Ancheyta predicts in its kinetic model are gasoline and LPG (which involves important light hydrocarbons such as C_3 and C_4) and also predict in its kinetic model dry gas and coke in which that the three last products may be founded and predicted independently by using other lumps **(Ancheyta *et al.,* 1999)**. **Sanchez *et al.* (2005)** proposed a five lump kinetic model with 10 kinetic parameters for moderate hydro cracking of heavy oils. The complexity of real feedstock suggests that models based on lumping theory will continue to be used for the study of hydro cracking reaction kinetics. However, more sophisticated and accurate approaches are required to provide better understanding and to ensure that the model is a reasonable representation of heavy oil hydro cracking kinetics **(Ancheyta *et al.,* 2005)**. However, the complexity of hydro cracking feed makes it enormously abstruse to characterize and describe its kinetics. One method to simplify this problem is to consider that's part of reactor divide into equivalent parts, the so called lumps or lumping technique, and then assume each class as independent entity **(Sadighi 2013)**. This modality is appealingly for kinetic modeling of complex mixtures, because of its simplicity **(Sadighi *et al.,* 2010)**. In addition, hydro cracking unit may be used for the industrial diesel hydro processing plant, which this unit involved from two hydrodesulphurization parts with one part of hydro cracking bed **(Eradal *et al.,* 2005)**.

Strategic vigilance is of vital importance in terms of making administrative quality decisions. It contributes to giving a general impression of consistency in government institutions, towards the aim of developing the development of community services. Therefore, it was necessary to consider greatly the decision to build oil projects, especially petroleum refineries. Because it has a great impact on spoiling the surrounding environment and badly damaged; which it is not easy to handle or control on it **(khlil 2019)**.

For the reason of indispensable idealities, this research depends on an ideal flow assumption to simplify the modality of a hydro cracking reactor model to predict the product yields and also predict the behavior of heavy oil in the hydro cracking reactor which depends mainly on the composition of feedstock.

Hydro cracking Reactor Modeling

In this investigation, the feed and product are lumped into heavy oil, vacuum oil, distillates, naphtha and gases to predict valuable products of a pilot plant reactor. (Figure 1) depicts the reaction

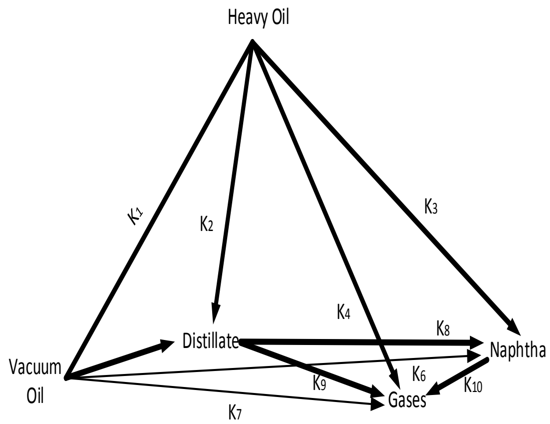

Figure (1): Kinetic model for the hydro cracking of heavy oils.

pathways; note that this kinetic model includes 5 lumps (heavy oil, vacuum oil, distillate, naphtha and gases) and 10 kinetic parameters. Some judgments are normally welcomed to reduce the model, without scarifying the accuracy. Upon close scrutiny of the system; the model can be reduced, requiring less kinetic parameters as shown in (Figure 2). In this work, the following assumptions have been made to simplify the model:

1. Hydro cracking is a first order hydro cracking reaction. Since hydrogen is present in excess.
2. Ideal trickle bed reactor, with plug flow.
3. Operation is at steady state.
4. Heat losses are negligible and reactor operates under isothermal conditions.

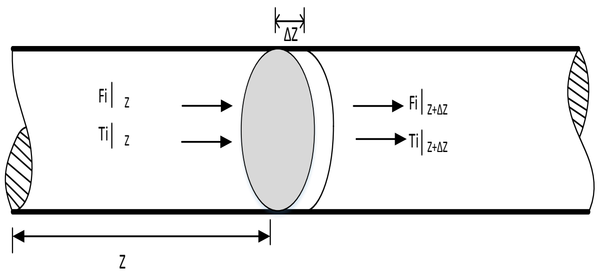

Figure (2): Schematic diagram of reactor.

Mass Balance

In (at particulars z location) - out (at z + Δz)+ net generation =accumulation.

Area * $F_{I,Z}$ – area * $F_{I,\Delta Z+\Delta Z}$+$\sum(r_f * Area * \Delta z - r_d * Area * z) = 0$

$Dividing\ by\ (area * \Delta z)$

$$\frac{F_{I,Z} - F_{I,Z+\Delta z}}{\Delta Z} + \varepsilon\,(r_f - r_d) = 0$$

$- [\frac{F_{I,Z} - F_{I,Z+\Delta z}}{\Delta Z}] = -\varepsilon\,(r_f - r_d)$

By taking$\lim_{\Delta z\to 0}$:

$- \frac{d\,F_{I,Z}}{dZ} = -\varepsilon\,(r_f - r_d)$

Dividing by -1, we get

$\frac{d\,F_{I,Z}}{dZ} = \varepsilon\,(r_f - r_d)$ ………(1)

The reaction rate of the model are:

$r_d = r_{ho}$

Heavy oil: $r_{ho} = -(k_1 + k_2 + k_3 + k_4)\, y_{ho}$

$r_f = r_{VO} + r_D + r_N + r_G$

Vacuum oil:

$r_{VO} = k_1 y_{ho} - (k_5 + k_6 + k_7)\, y_{Vo}$

Distillates:

$r_D = K_2\, y_{ho} - K_5\, y_{vo} - (K_8 + K_9) * y_D$

Naphtha:

$r_N = K_3\, y_{ho} + K_6\, y_{vo} + K_8\, y_D - K_{10}\, y_N$

Gases:

$r_G = K_4\, y_{ho} + K_7\, y_{vo} + K_{10}\, y_N$

Hence:

$F_{I,Z} = y_I\,(W_{IZ} + W_{IJ})$ ………(2)

$y_I\,(W_{IZ} + W_{IJ}) = UC_I$ ………(3)

Sub 3 into 2 gives: -

$F_{I,Z} = UC_I$ …….(4)

By differentiate equation (4) gives:

$\frac{d\,F_{I,Z}}{d\,z} = u\,\frac{d\,C_i}{d\,z}$ …..(5)

sub eq. (5) into eq. (1)

$u\,\frac{d\,C_I}{d\,z} = \varepsilon\,(K_{fj}C_j - K_{dI}C_I)$

By dividing on (C_T) we get

$u\,\frac{d\,y_I}{d\,z} = \varepsilon\,(K_{fj}y_j - K_{dI}y_I)$

Five first order differential equations were solved by using 2nd order Runge – kutta method and implemented in MATLAB 6.1.

Where:

z	Axial distance, m
ε	Liquid hold up
r_{ho}	Reaction rate of heavy oil(wtfraction/hr)
r_{vo}	Reaction rate of vacuum oil

(wt fraction/hr)

r_D Reaction rate of distillates (wt fraction/hr)

r_N Reaction rate of naphtha (wt fraction/hr)

r_G Reaction rate of gases (wt fraction/hr)

K_1 first –order rate constant for the hydrocracking of heavy oil to vacuum oil(hr^{-1})

K_2 first –order rate constant for the hydrocracking of heavy oil to distillates(hr^{-1})

K_3 first –order rate constant for the hydrocracking of heavy oil to naphtha (hr^{-1})

K_4 first –order rate constant for the hydrocracking of heavy oil to gases (hr^{-1})

K_5 first –order rate constant for the hydrocracking of vacuum oil to distillates (hr^{-1})

K_6 first –order rate constant for the hydrocracking of vacuum oil to naphtha (hr^{-1})

K_7 first –order rate constant for the hydrocracking of vacuum oil to gases (hr^{-1})

K_8 first –order rate constant for the hydrocracking of distillates to naphtha (hr^{-1})

K_9 first –order rate constant for the hydrocracking of distillates to gases(hr^{-1})

K_{10} first –order rate constant for the hydrocracking of naphtha to gases (hr^{-1})

K_f Rate constant of reaction for formatiom,1/hr

K_d Rate constant of reaction for dissociation,1/hr.

F molar flowrate (mole/hr)

$r_f$rate constant for formation (1/hr)

r_d rate constant for dissociation (1/hr)

Result and Discussion

From (Figure 3, 4 and 5), it is clearly that as the feed velocity is reduced and consequently the reaction severity is increased, these curves are moved to the right, which means that high boiling point molecules are converted into lighter ones. Conversion of heavy oil to various products was higher at lower feed velocity which is shown by (Figure 3, 4, 6 and 7). There was predominant decrease in concentration of heavy oil as in (Figure 5). From the (Figure 8 and 9) notice the reaction selectivity guided towards production of vacuum oil and distillate. That explicitly from the distinctness of the yield for each product (Figure 9). Naphtha and lighter products is only slightly higher than that of the original feed. This behavior has two explanations: (1) Naphtha and gases formation rates are almost equal the naphtha hydro cracking rate or (2) Naphtha and gases formation from heavy fractions is insignificant. To increase the amount of desired products we should increase the rate of all reactions in this unit. possible by increasing the rate of all reactions, from the (Figure 10, 11, 13 and 14) showed increase of temperature well increase the amount of desired products with remarkable decrease in amount of heavy oil (Figure 12) with increasing the temperature, and from the (Figure 10, 11, 13 and 14), showed that the optimum temperature it was 430°C which gave the best recovers of the desired products.

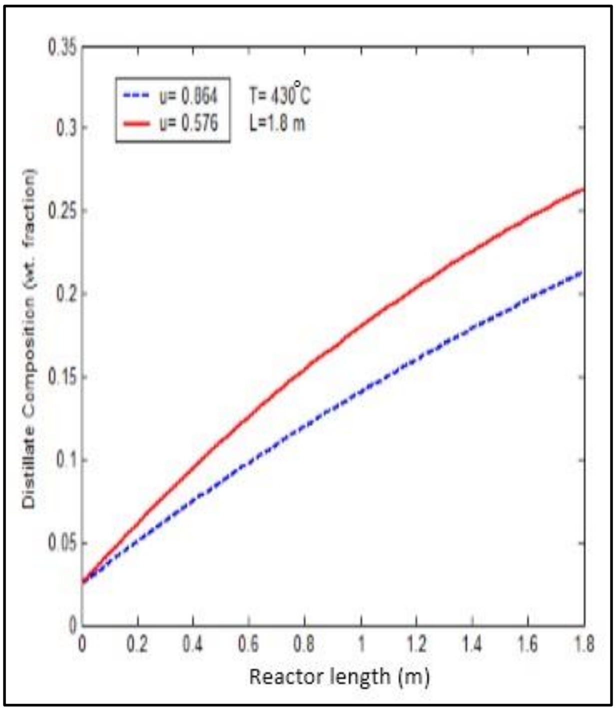

Figure (3): Effect of feed velocity on Distillate Fraction interms of reactor height (at operating temperature = 430°C).

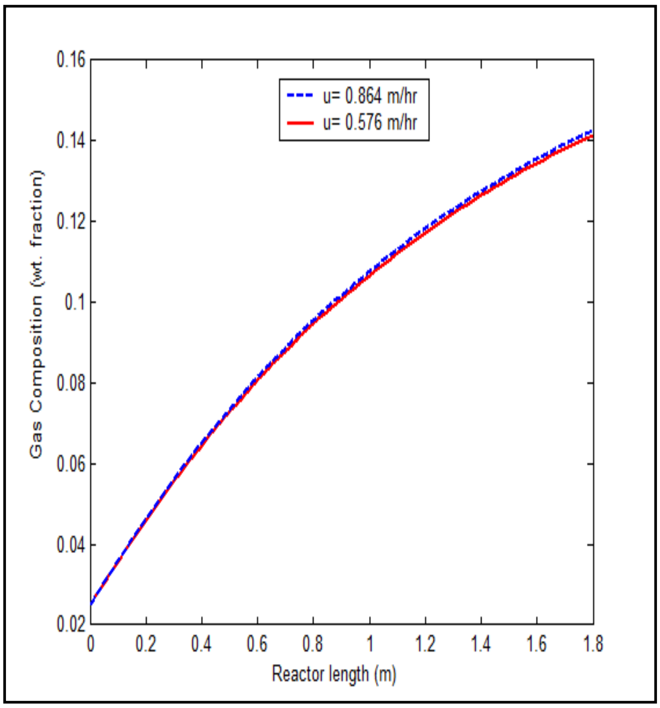

Figure (4): Effect of feed velocity on Gas fraction in terms of reactor height (at operating temperature =430°C).

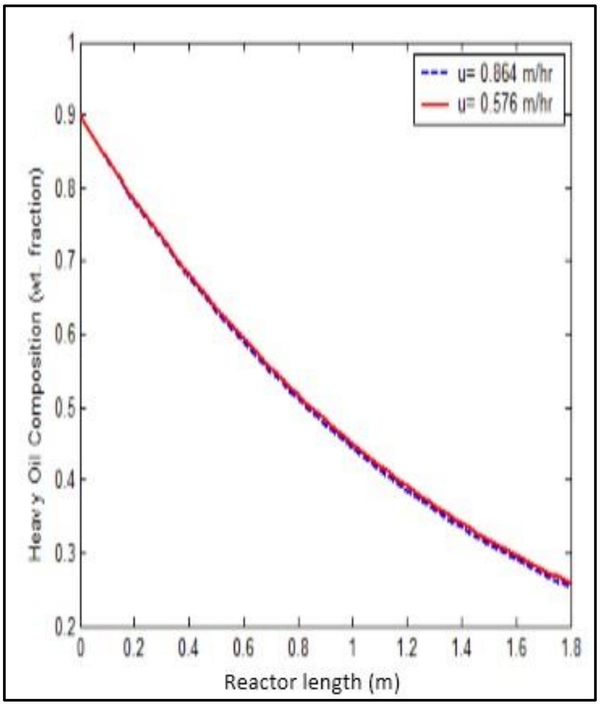

Figure (5): Effect of feed velocity on Heavy Oil fraction in terms of reactor height (at operating temperature = 430°C).

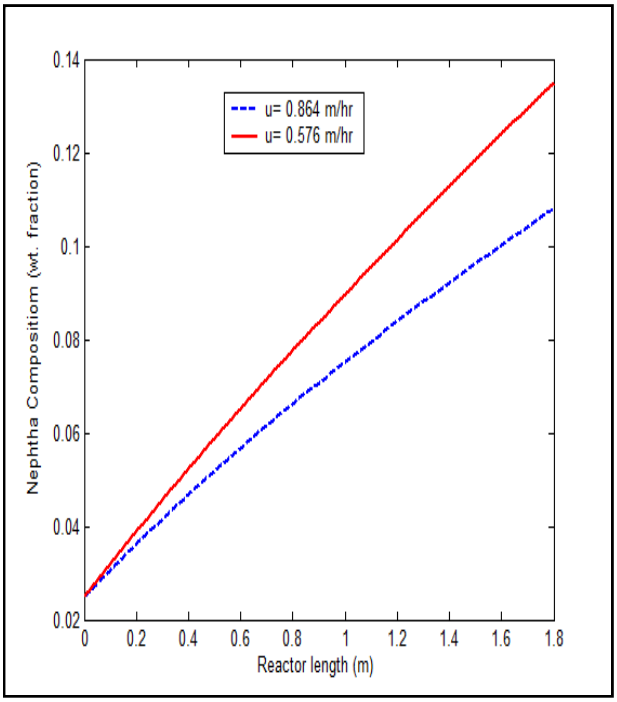

Figure (6): Effect of feed velocity on Naphtha fraction in terms of reactor height (at operating temperature = 430°C).

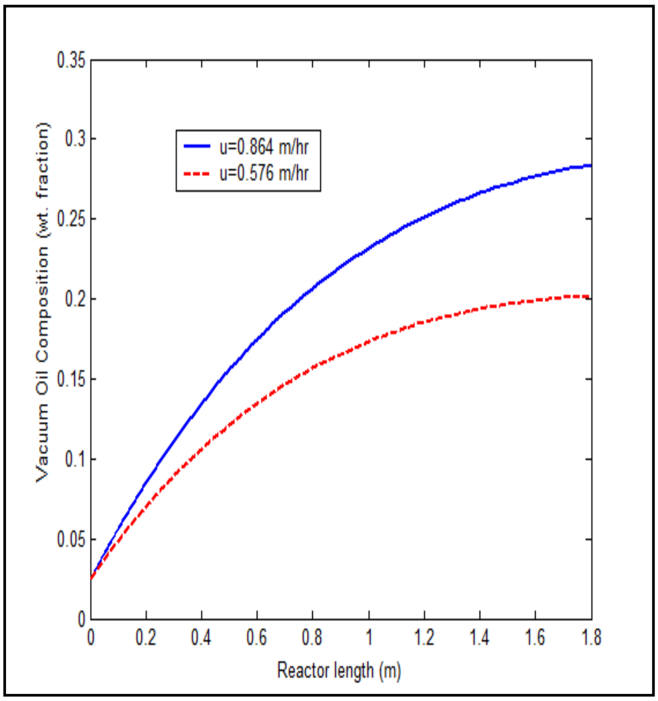

Figure (7): Effect of feed velocity on Vacuum Oil fraction in terms of reactor height (at operating temperature = 430 °C).

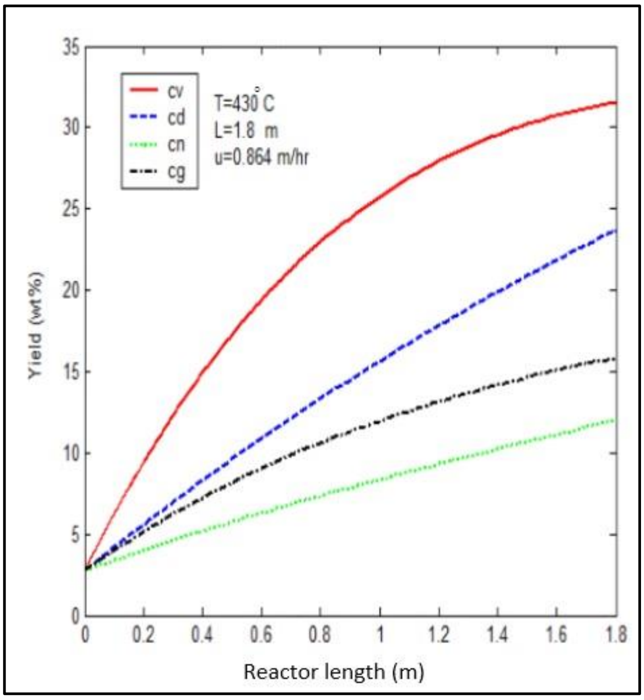

Figure (8): Effect of feed velocity on the yield of different products along reactor length (at operating temperature = 430°C and feed velocity = 0.864 m/hr), (cv= vacuum, cd= distillate, cn= naphtha, cg= gases).

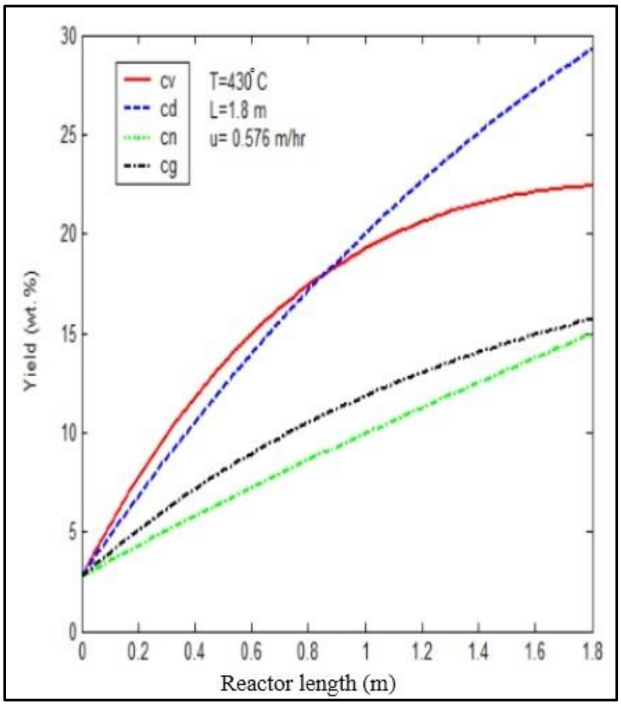

Figure (9): Effect of feed velocity on the yield of different products along reactor length (at operating temperature = 430 °C and feed velocity = 0.576 m/hr)(cv= vacuum, cd= distillate, cn= naphtha, cg= gases).

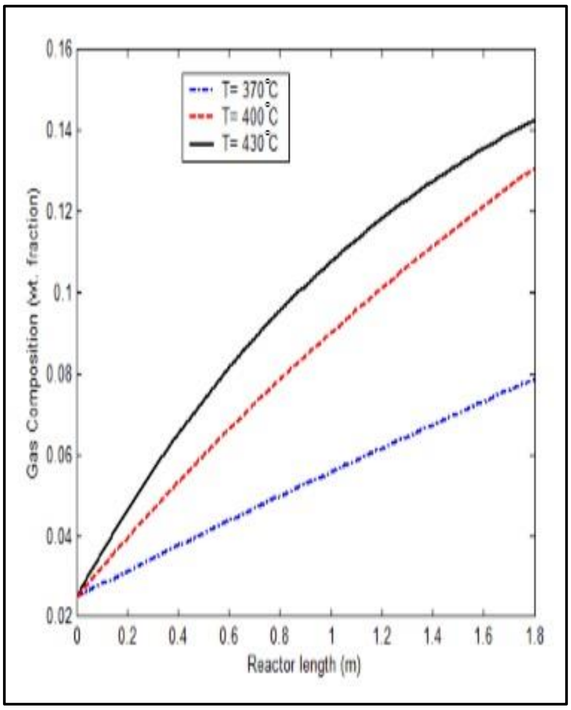

Figure (10): Effect of operating temperature on Gases as product along reactor length (at feed velocity = 0.864 m /hr).

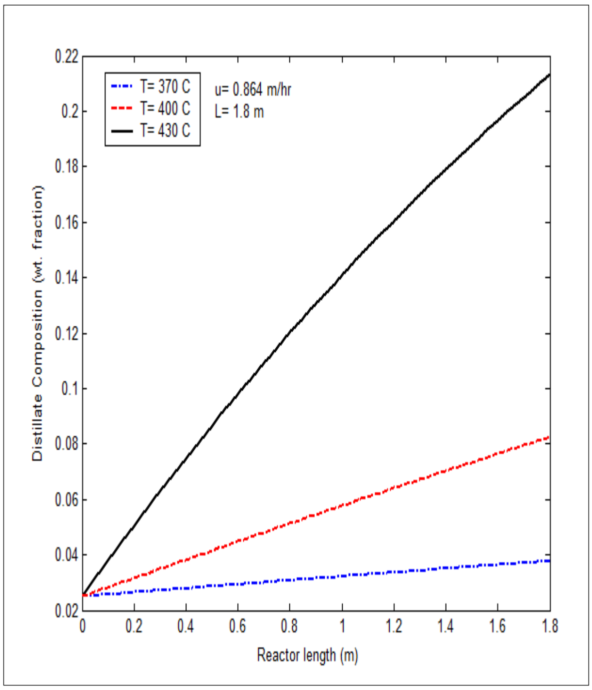

Figure (11): Effect of operating temperature on Distillate as product along reactor length (at feed velocity = 0.864 m /hr).

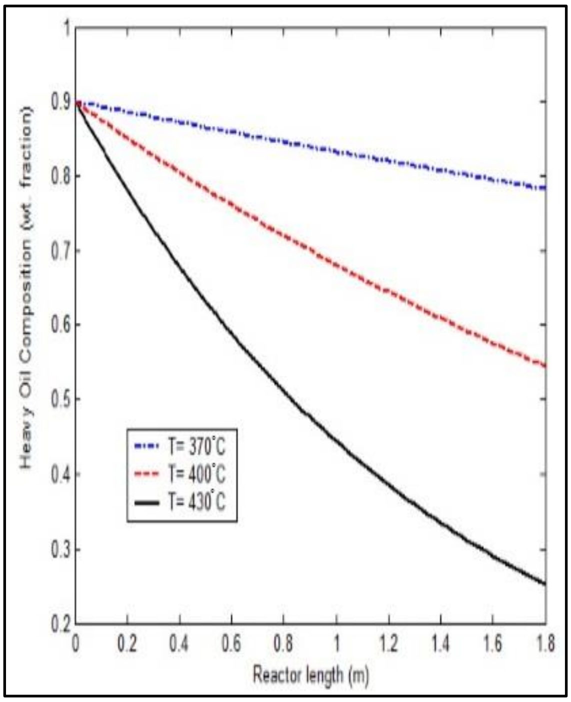

Figure (12): Effect of operating temperature on Heavy Oil as product along reactor length (at feed velocity = 0.864 m /hr).

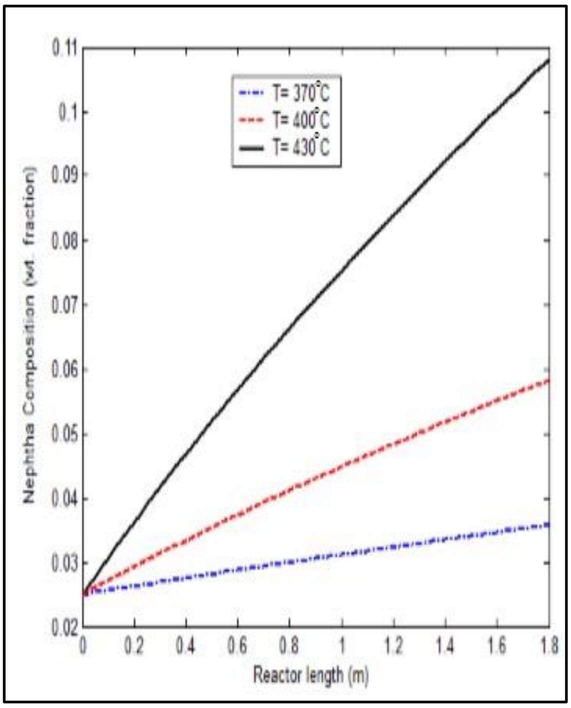

Figure (13): Effect of operating temperature on Naphtha as product(at feed velocity = 0864m/hr).

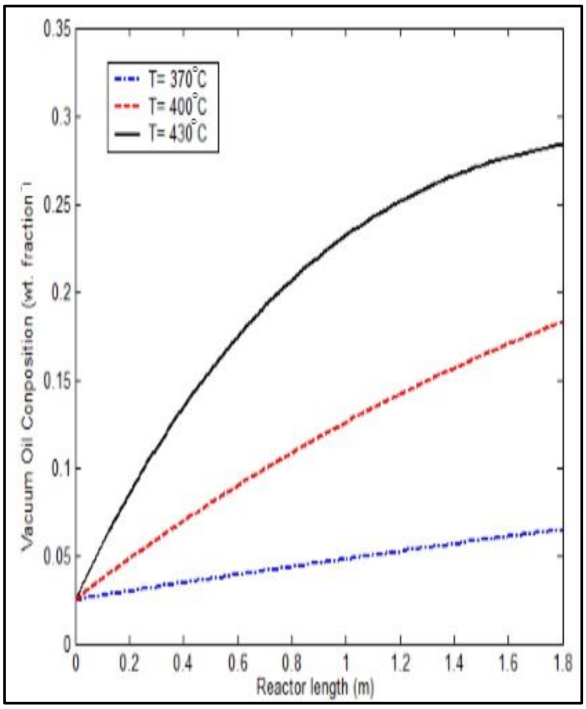

Figure (14): Effect of operating temperature on Vacuum Oil as product (at feed velocity = 0.864 m/hr).

Conclusion

In this study a five lump kinetic model was taken in order to apply for heavy oils at the reactor of hydro cracking. This model is capable of predicting the production of unconverted heavy oil, vacuum oil, distillates, naphtha, and gases. The hydro cracking reactor was quite sensitive to operating temperature and fresh feed flow rate. The production of important products such as vacuum oil and distillates could be ameliorated by restrictions on the temperature and feed velocity, to get better gratifying trammels due to conspicuous the redounding of feed velocity and temperature on the mechanism of chemical reactions occurring in hydro cracking, thus increasing the overall conversion, this also increases the production rates of low value products, the temperature has greatly run away, constraints on the temperature should be considered.

Recommendations

1. A hydro cracking reactor enhances to increase the desired production with respect to least reduction in the hydrogen and fuel gas consumption.
2. This work can be extended to unsteady state analysis of reactor.
3. This model was solved by assuming that reactor was isothermally, so this work can be extended to thermal analysis.
4. The present lumped model can also be simulated in HYSYS.
5. Investigating the effects of catalyst deactivation on model parameters.

REFERNCE

I. Ancheyta, J., Lopez, F. & Grewal, R. (1999). 5-Lump kinetic model for gas oil catalytic cracking. *Applied Catalysis*, 177, 227-235.

II. Ancheyta, J., Sanchez, S. & Rodriguez, M. (2005). The kinetic modeling of hydro cracking of heavy oil fractions: a review. *Journal of Catalysis*, 109, 76-92.

III. Khlil, A, S. (2019). Strategic vigilance and its impact on the quality of management decision survey study in the supreme judicial council. *Iraqi Journal of Market Reseach and Consumer Protection*, 11, 2, 1-16.

IV. Becker, P., Celse, B., Gruillaume, D. & Dulot, H. (2016). Comparing hydro cracking models: continuous lumping vs. single events. *The Science and Technology of Fuel and Energy Journal*. 165. 306-315.

V. Erdal, A., Ayse, D., Hasan, S., Yaman, A. & Ummuhan, C. (2005). Dynamic modeling of an industrial diesel hydro processing plant by the method of continuous lumping. *Computer and Chemical Engineering Journal*. 82, 44-54.

VI. Ignacio, E., Miguel, A. & Jorge, A. (2010). Modeling the effect of pressure and temperature on the hydro cracking of heavy crude oil by the continuous kinetic lumping approach. *Applied Catalyst*, 382, 205-212.

VII. Sadighi, S. (2013). Modeling a vacuum gas oil hydro cracking reactor using axial dispersion lumped kinetics. *Petroleum and Coal*, 55(3), 156-168.

VIII. Sadighi, S., Ahmed, A. & Rashidzadeh, M. (2010). 4-Lump kinetic model for vacuum gas oil hydrocracker involving hydrogen consumption. *Korean Journal of Chemical Engineering*, 27(4), 1099-1108.

IX. Sadighi, S., Ahmed, A. & Masoudian, S. (2012). Effect of lump partitioning on the accuracy of a commercial vacuum gas oil hydro cracking model. *International Journal of Chemical Reaction Engineering*, 10(A16), 1-21.

X. Sanchez, S., Rodriguez, M. & Ancheyta, J. (2005). Kinetic model for moderate hydro cracking of heavy oils. *Industrial Engineering Chemical Research*, 44, 9409-9413.

XI. Valvarasu, G., Bhaskar, M. & Sairam, B. (2005). A four lump kinetic model for the simulation of the hydro cracking process. *Petroleum Science and Technology*, 23, 1323-1332.