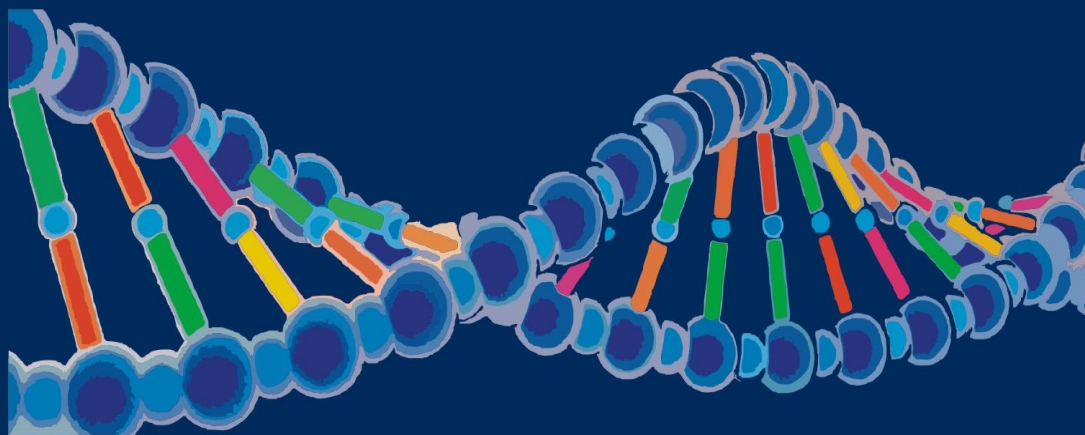


SCIENCE  
THE INDIAN  
JOURNAL  
OF RESEARCH  
ANVIKSHIKI

Bi-Monthly International Journal of all Research



Volume-9-10

Number-6 & 1

November-2015 & January 2016

ISSN 0973-9777  
GISI Impact Factor 2.4620  
Volume-9-10, Number-6 & 1  
November-2015 & January 2016



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mpasvo Press, Varanasi, U.P. India. A Subscription to The Indian Journal of Research : Anvikshiki Comprises 6 Issues in Hindi and  
6 in English and 3 Extra Issues. Prices include Postage by Surface mail, or For Subscription in the India by Speed Post.  
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Office Time : 3-5 P.M. (Sunday off)

**Journal set by :** Maheshwar Shukla, maheshwar.shukla@rediffmail.com

**Printed by :** Mpasvo Press

**Date of Publication :** 1 January 2016



**Maneesha Publication**

(Letter No. V-34564, Reg. 533/2007-2008)

B-32/16-A-2/1, Gopalkunj, Nariya, Lanka

Varanasi, U.P., India

# Anvikshiki

## The Indian Journal of Research

Volume 9-10 Number 6&1 November 2015 & January 2016

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PRINT ISSN 0973-9777, WEBSITE ISSN 0973-9777

## MODELLING AND SIMULATION OF TRICKLE BED REACTOR FOR HYDROTREATING OF CRUDE OIL

AKANKSHA PATHAK\*

### *Declaration*

The Declaration of the author for publication of Research Paper in The Indian Journal of Research Anvikshiki ISSN 0973-9777 Bi-monthly International Journal of all Research: I, *Akanksha Pathak* the author of the research paper entitled MODELLING AND SIMULATION OF TRICKLE BED REACTOR FOR HYDROTREATING OF CRUDE OIL declare that , I take the responsibility of the content and material of my paper as I myself have written it and also have read the manuscript of my paper carefully. Also, I hereby give my consent to publish my paper in Anvikshiki journal , This research paper is my original work and no part of it or it's similar version is published or has been sent for publication anywhere else. I authorise the Editorial Board of the Journal to modify and edit the manuscript. I also give my consent to the Editor of Anvikshiki Journal to own the copyright of my research paper.

### *Abstract*

*Hydrotreating (HDT) of crude oil is one of the most difficult tasks in the petroleum refining industries that have not been considered largely in the literature . The accurate calculations of kinetic models of the relevant reaction scheme are required for obtaining helpful models for HDT reactions, which can be confidently used for reactor design, operating and control. In this work, an optimization technique is employed .To evaluate the best kinetic models of a trickle bed reactor (TBR) process utilized for hydrodenitrogenation(HDN) and hydrodemetallization (HDM) that includes hydrodevanadization (HDV) and hydrodenickelation (HDNi) of crude oil based on pilot plant experiments. The minimization of the sum of the squared errors (SSE) between the experimental and estimated concentrations of nitrogen (N), vanadium(V) and nickel (Ni) compounds in the products is used as an objective function in the optimization problem to determine the kinetic parameters.*

*The commercial cobalt–molybdenum on alumina (Co–Mo/c-Al<sub>2</sub>O<sub>3</sub>) was used as a catalyst in the trickle bed for hydrotreating process and the data for these processes was collected from the literature. A three-phase heterogeneous model based on two–film theory is developed to describe the behaviour of crude oil hydroprocessing in a pilot–plant trickle bed reactor (TBR) system. The hydroprocessing reactions have been modelled by power law kinetics with respect to nitrogen, vanadium and nickel compounds, and with respect to hydrogen. Here we have used MATLAB for modelling, simulation and parameter estimation via optimization using solver and data analysis kit. The model simulations results were found to agree well with the experiments carried out in a wide range of the studied operating conditions. The model is employed to predict the concentration profiles of hydrogen, nitrogen, vanadium and nickel along the catalyst bed length in three phases.*

**Keywords:** Hydrodenitrogenation, hydrodemetallization , trickle-bed reactor, mathematical modelling, parameter estimation

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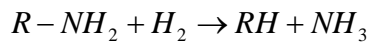
### 1. Introduction

Hydrotreating process is a conversion process driven by the catalytic reaction of hydrogen with the feedstock to produce higher-value hydrocarbon products and to reduce the content of impurities, such as nitrogen and metallic compounds from crude oil or oil fractions at high temperatures and hydrogen pressures through converting nitrogen in nitrogenic compounds to ammonia, respectively. Moreover there is the conversion of unsaturated hydrocarbon compounds such as olefins to saturated hydrocarbonic compounds.

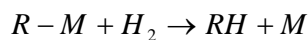
Hydrotreating processes have been studied by many investigators for the purpose of obtaining a large economic benefit by reducing the undesirable compounds in petroleum fractions. Hydrodenitrogenation (HDN) processes is the process to convert nitrogen compounds in the feedstock to denitrogenated hydrocarbon products such as ammonia (NH<sub>3</sub>) etc. Hydrodemetallization reactions (HDM) reaction is thermo catalytic and it produces metallic sulfides such as NiS and V<sub>3</sub>S<sub>4</sub>.

The general hydrotreating reactions can be expressed as follows :

HDN



HDM



Where M-Ni,V,N

#### 1.1 Process Variables of HDT Process

The operating conditions are determined by the feedstock type, the required product level, and the purity and availability of hydrogen in addition to economic considerations. There are four process variables frequently reported in the literature as the most important in hydrotreating operations: reaction temperature, liquid hourly space velocity (LHSV), hydrogen partial pressure and hydrogen to oil ratio (H<sub>2</sub>/Oil) ratio.

#### Temperature

Temperature plays a significant role in the HDT process. An increase in reaction temperature can substantially enhance the rate of catalytic reaction and hence increase the sulfur, nitrogen, asphaltene and metal removal. In addition to catalytic improvement, temperature increase may significantly enhance the thermal cracking. The rate of heavy hydrocarbons will be decreased when the reaction temperature increases. On the other hand, the rate of diffusion inside the active site of the catalyst will increase and as a result the rate of reaction will be increased .

The best range of temperature used in the refineries lies between 553K and 683K (except heavy vacuum residue), where under 553K the reaction rates tend to be slow and above 683K there is undesirable side reaction. At temperatures above 683K, the activity of the catalyst used will decrease due to coke formation that deposits on the catalyst.

### *Pressure*

Hydrogen partial pressure is another parameter that mainly affects the rate of reaction by promoting the reaction between hydrogen and feedstock compounds. The performance of any hydroprocessing reactor and process is limited by the hydrogen partial pressure at the inlet to the reactor. More specifically, the partial pressure of hydrogen has a direct influence on the rate of reaction of HDS, HDN, HDAs and HDM of the feedstock. In addition, the system pressure impacts both the degree of hydrogenation of unsaturated compounds in the feedstock as well as the reaction rate of hydrocarbon cracking. Refinery experience indicates that the HDT processes conducted at higher partial pressure of hydrogen will produce products with lower sulfur, nitrogen and aromatics contents. The choice of operating partial pressure of hydrogen must therefore be made with care in order to ensure that the process operates under HDT conditions and to prevent high deactivation of catalyst used.

### *Liquid Hourly Space Velocity (LHSV)*

LHSV can be defined as the ratio of the feed volumetric flow rate to the catalyst volume. The reciprocal of liquid hourly space velocity gives the residence time of feedstock along the catalyst bed. Although the volume of catalyst for the HDT process will be constant, the liquid hourly space velocity will vary directly with the rate of feedstock. A decrease in LHSV will cause an increase in feed contact time (residence time) in catalyst. On the other hand, a decrease in the LHSV will generally bring an increase in the extent of the HDS, HDN, HDM, HDAs and HDC processes and as a result, increase the reaction severity and the efficiency of the hydrotreating processes.

### *Gas Rates ( $H_2$ /Oil ratio)*

The choice of gas flow rate is governed by economic considerations. Recycle is utilized to maintain the  $H_2$  partial pressure and the physical contact of the hydrogen with the catalyst and hydrocarbon for ensuring adequate conversion and impurities removal. To make the process economically feasible, the unused hydrogen is recycled back to the reactor.

### *1.2. Trickle Bed Reactors (TBRs)*

A trickle-bed expression is generally used to a reactor in which a gas phase (hydrogen frequently) and a liquid phase (feedstock oil) flow co-currently downward through a solid fixed particles (catalyst-bed), where the reaction take place. The older term used was "trickling filter", that has long been utilized for organic removal from wastewater streams by the action of aerobic bacteria. The trickle bed reactor consists of a cylindrical column in which a fixed bed of catalyst particles is randomly dumped.

Trickle-bed reactors with co-current downflow are widely used in hydrotreating operations. This type of TBR has many features, where the liquid flow approaches plug flow behavior with very low catalyst loss (i.e. the catalyst is effectively wetted). This feature is very significant when costly catalyst is utilized. These factors allow high conversion to be achieved in a single reactor. Also, the volume ratio of liquid to solid (liquid hold-up) in this type of reactor is low; thus minimizing the homogeneous reaction (less occurrences of homogeneous side-reactions) and this could be significant in the HDT reaction. The objectives of the work is to carry out the literature survey on the modelling, simulation

and optimization of trickle bed reactor (TBR) processes and to develop the best kinetic models for HDN, HDV and HDNi reactions which can be accurately applied to design of reactor, operation and control and further to determine the best kinetic parameters and to validate the model at different operating conditions for obtaining helpful models for HDT reactions, which further can be implemented for reactor design, operation and control.

## 2. Methodology

The main HDT reactions considered in this work are hydrodenitrogenation (HDN) and hydrodemetallization (includes hydrodevanadization (HDV)). These reactions were carried out in a continuous flow trickle bed reactor (TBR) using crude oil as a feedstock and cobalt–molybdenum as a catalyst. The data obtained from the literature are used to develop the kinetic models that can represent the HDN, HDV, HDNi, reactions to determine kinetic parameters and to validate the model under various operating conditions. The Mathematical modelling of the HDT process is a difficult task due to the complex physical and chemical changes that the feed undergoes, along with the mass transfer phenomena in the reaction system. Kinetic aspects are a major factor of reactor modelling, but in this case, the conversion of a large amount of nitrogen, vanadium and nickel compounds make it a huge problem. The following assumptions based on the literature survey were used to create the simple mathematical models for HDT processes :

- No radial concentrations gradients,
- Steady–state operation of the reactor,
- One-dimensional heterogeneous model,
- Isothermal and constant pressure operation of the reactor, and
- The effect of catalyst deactivation on kinetic parameters is negligible.

### 2.1. Mathematical Model of TBR for HDT Reactions

An essential stage in the improvement of any model is the formulation of the appropriate mass and energy balance equations. To these should be added suitable kinetic equations of chemical reaction rates, rates of mass and heat transfer and equations representing process property changes. The basic mathematical model can be provided by combination of these relationships.

A three–phase heterogeneous model is used for describing the behaviour of pilot-plant trickle-bed reactors applied to the HDT of crude oil. The model is based upon two-film theory and includes correlations for calculating mass–transfer coefficients, oil density, Henry’s coefficients, solubility of hydrogen, oil viscosity, diffusivity, molar volume, specific surface area, etc. under the operating conditions, using information presented in the literature.

### *Model Equations*

The reactor model considers the main crude oil hydrotreating reactions (HDN, HDV and HDNi) that take place on the catalyst surface. The concentration profile of reactants and products in a trickle bed reactor model is shown schematically in Figure 1.

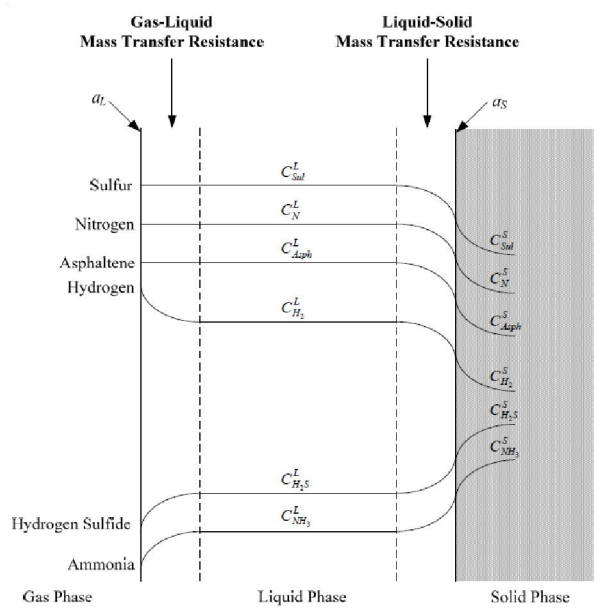


Figure 3 : Concentration profile in Trickle bed reactor

The mass transfer of reactants and products in the heterogeneous model are taken into account in all the phases. The mathematical model equations are based on the transfer coefficients of the process at gas–liquid, liquid–solid interfaces and also involve the mass transfer rates in addition to distribution of reactants and products in various phases. The mass balance for each compound in each phase can be described as follows

### Mass Balance Equations in Gas Phase

Hydrogen:

$$\frac{dP_{H_2}}{dz} = \frac{RT}{u_g} k_{H_2}^L a_L \left( \frac{P_{H_2}}{h_{H_2}} - C_{H_2}^L \right)$$

Above equation include a system of ordinary differential equations (ODEs) that relate the partial pressures of H<sub>2</sub> to the mass transfer of the compounds across the gas–liquid interface. These equations can be solved to give partial pressure profiles of hydrogen and hydrogen sulfide along the catalyst bed length when the concentrations of these compounds in the liquid phase are known. The differential equations of mass balance for the concentrations of hydrogen in the *liquid phase* can be written by equating the concentrations gradient to the mass transfer of H<sub>2</sub> across the gas–liquid and liquid–solid as follows

$$\frac{dC_{H_2}^L}{dz} = \frac{1}{u_L} \left[ k_{H_2}^L a_L \left( \frac{P_{H_2}^L}{h_{H_2}} - C_{H_2}^L \right) - k_{H_2}^S a_S (C_{H_2}^L - C_{H_2}^S) \right]$$

$$\frac{dC_i^L}{dz} = \frac{1}{u_L} k_i^S a_S (C_i^L - C_i^S)$$

Where i=N, V, Ni



### Mass Balance Equations in Solid Phase

The solution of the above equations requires surface concentrations of H<sub>2</sub>, N, V and Ni. At steady-state, the compounds transported between the liquid phase and the solid phase (on the surface of the catalyst) are consumed or produced through the chemical reaction. By equating the liquid–solid interfacial mass transfer of H<sub>2</sub>, N, V and Ni components with their reaction rates, the following equations were obtained:

Hydrogen-

$$k_{H_2}^S a_s (C_{H_2}^L - C_{H_2}^S) = \rho_B \sum \eta_j r_j$$

Nitrogen-

$$k_N^S a_s (C_N^L - C_N^S) = \rho_B \eta_{HDN} r_{HDN}$$

VANADIUM-

$$k_V^S a_s (C_V^L - C_V^S) = \rho_B \eta_{HDV} r_{HDV}$$

NICKEL

$$k_{Ni}^S a_s (C_{Ni}^L - C_{Ni}^S) = \rho_B \eta_{HDNi} r_{HDNi}$$

### Chemical Reaction Rate

Developing kinetic models for crude oil hydrotreating reactions is not a simple task because of the complexities of crude oil composition and its analysis. Modelling of such reactions is a hard task due to the large numbers of components of crude oil. For such a complex feed, the reaction rate equation is generally lumped into a single power law reaction. HDN, HDV and HDNi reactions are modelled by the power law models with respect to the concentration of nitrogen, vanadium and nickel and with hydrogen as follows:

$$r_j = K_j (C_i^S)^{n_j} (C_{H_2}^S)^{m_j}$$

$$K_j = A_j^0 \exp\left(\frac{EA_j}{RT}\right)$$

i = NI, V, N.

*Gas–Liquid Mass Transfer Coefficients:* The correlations used for estimating the gas–liquid mass transfer coefficients are

$$\text{Hydrogen: } \frac{K_{H_2}^L a_L}{D_{H_2}^L} = 7 \left(\frac{G_L}{\mu_L}\right)^{0.4} \left(\frac{\mu_L}{\rho_L D_{H_2}^L}\right)^{0.5}$$

*Liquid–Solid Mass Transfer Coefficients:* The liquid–solid mass transfer coefficients can be calculated from the Van Krevelen–

Krekels equation as follows:

$$\text{Hydrogen: } \frac{K_{H_2}^S}{D_{H_2}^L a_s} = 1.8 \left(\frac{G_L}{a_s \mu_L}\right)^{0.5} \left(\frac{\mu_L}{\rho_L D_{H_2}^L}\right)^{1/3}$$

Molecular Diffusivity : To determine the liquid–solid and gas–liquid mass transfer coefficients, it is necessary to know the molecular diffusivity of  $H_2$ , N, V and Ni in the liquid, which can be calculated by a Tyn-calus correlation:

$$D_i^L = 8.93 \times 10^{-8} \frac{v_L^{0.267} T}{v_i^{0.433} \mu_L}$$

i=H<sub>2</sub>,N,Ni,V

*Henry's Law Coefficient* : Henry's coefficients for  $H_2$  and  $H_2S$  can be calculated from solubility coefficients

$$\text{Hydrogen: } h_{H_2} = \frac{V_{H_2}}{\lambda_{H_2} \rho_L}$$

$$\lambda_{H_2} = 0.559729 + 0.42947$$

*Oil Viscosity* : Glaso's equation, Shokri and Zarrinpashne (2006) is used a generalized mathematical equation for oil viscosity. The equation has the following form

$$\mu_L = 3.141 \times 10^{10} (T - 460)^{-3.444} [\log_{10}(API)]^a$$

$$a = 10.313 [\log_{10}(T - 460)] - 36.447$$

$$API = \frac{141.5}{sp \cdot gr_{15.5}} - 131.5$$

*Effectiveness Factor ( $\eta$ )* : Internal diffusion limitations are usually expressed in terms of the catalyst effectiveness factor ( $\eta$ ). It has been noted that the chemical reaction rate decreases with increasing particle size. In the literature, the effectiveness factor has been reported to be in the range of 0.0057 to 1. Because the particle size of the catalyst is small, the effectiveness factor ( $\zeta$ ) can be estimated as function of Thiele Modulus

$$\eta_i = \frac{\tanh \phi_i}{\phi_i}$$

i =HDN,HDV,HDNi

$$\text{where, } \phi_i = \frac{V_p}{S_p} \left[ \left( \frac{n_i + 1}{2} \right) \left( \frac{K_i C_j^{S(n_i-1)} \rho_P}{De_j} \right) \right]$$

i=HDN,HDNi,HDV, J=Ni,V,N

Where

$$De_i = \frac{\theta}{\tau} \left( \frac{1}{\left( \frac{1}{D_j^L} \right) + \left( \frac{1}{D_{K_j}} \right)} \right)$$

$$r_g = \frac{2\theta}{S_g \rho_p} \quad \text{and}$$

$$\theta = \rho_p V_g$$

3. Results and Discussion

A comparison between experimental results and model prediction results for HDN, HDV and HDNi of crude oil were plotted in Figs. 7–9. As can be seen from the results, the model was found to simulate the performance of the pilot plant TBR very good agreement in the range of operating conditions

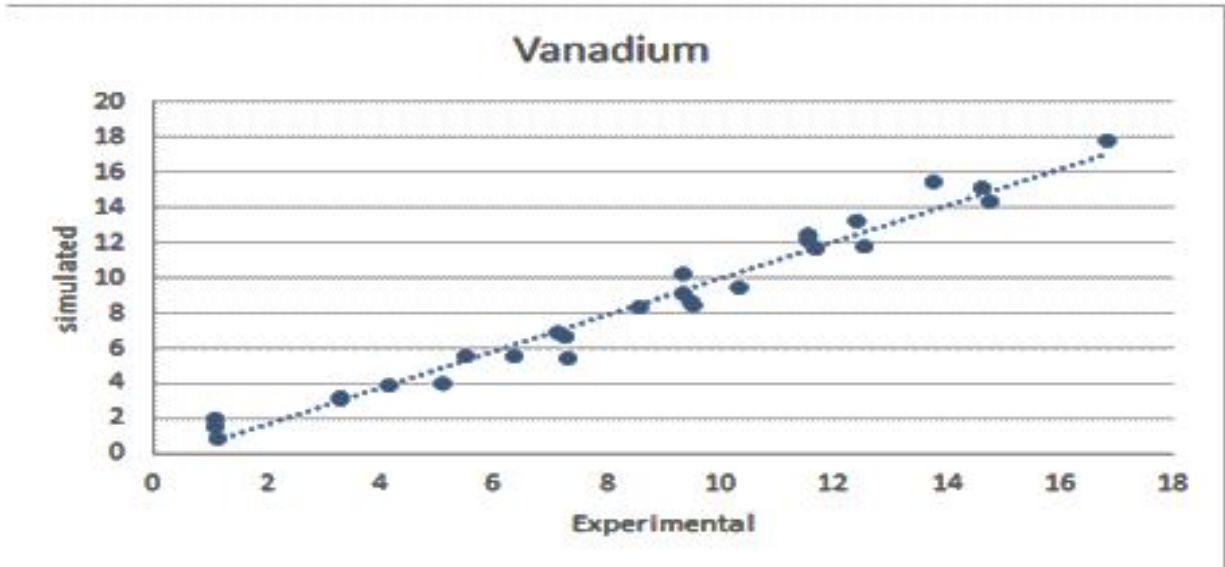


Figure 7: Comparison between simulated and experimental result of Vanadium

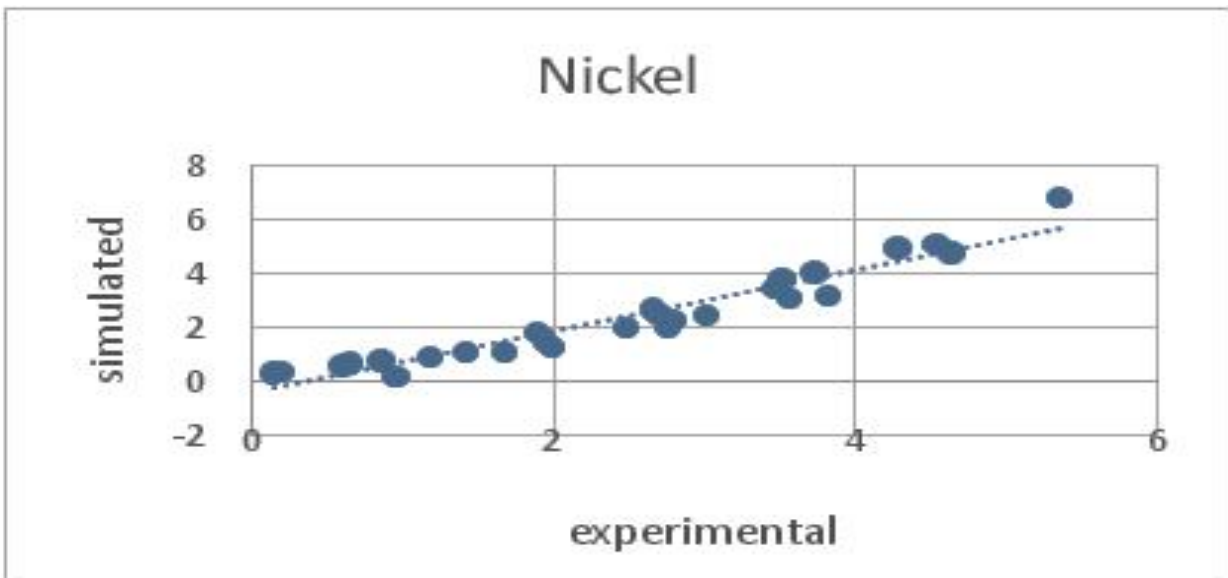


Figure 8: Comparison between simulated and experimental result of Nickel

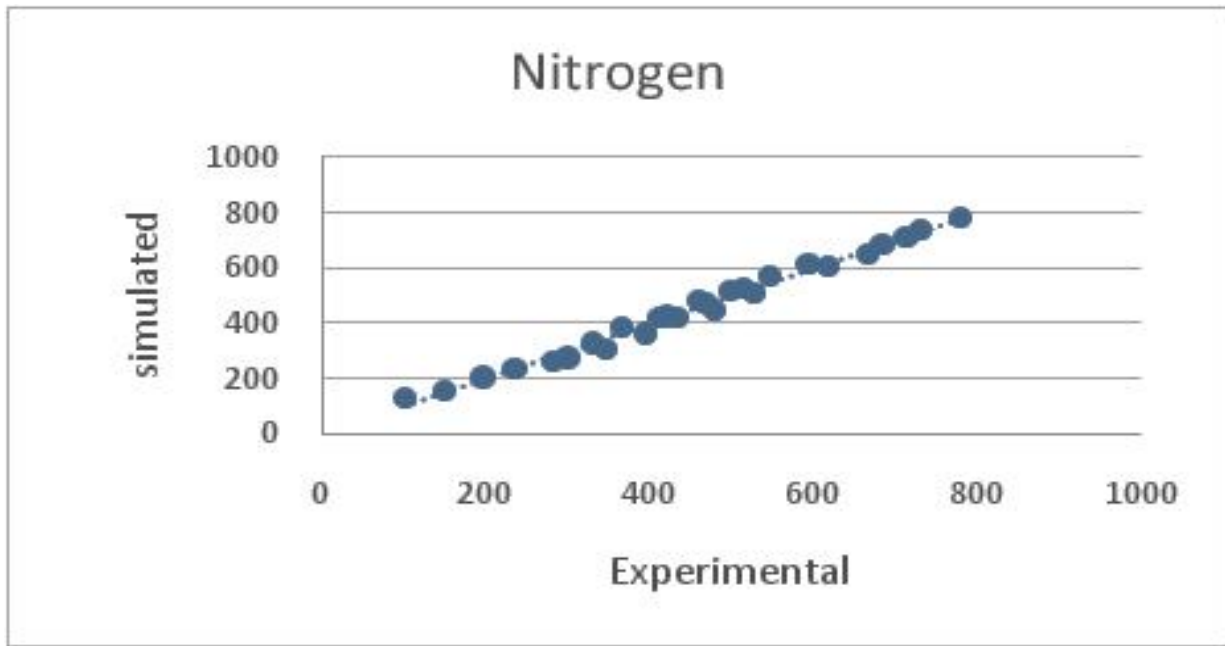


Figure 9: Comparison between simulated and experimental result of Nitrogen

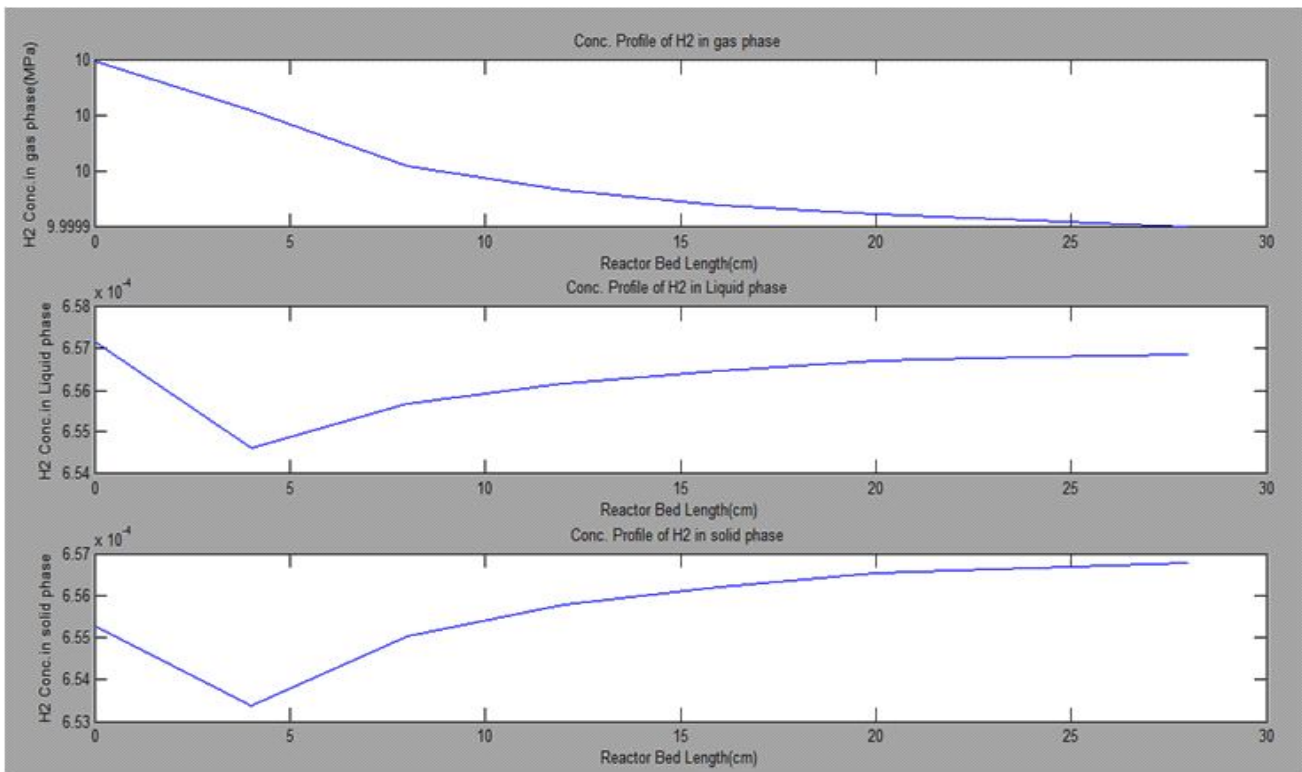


Figure 10 : Variation of Hydrogen concentration along reactor length

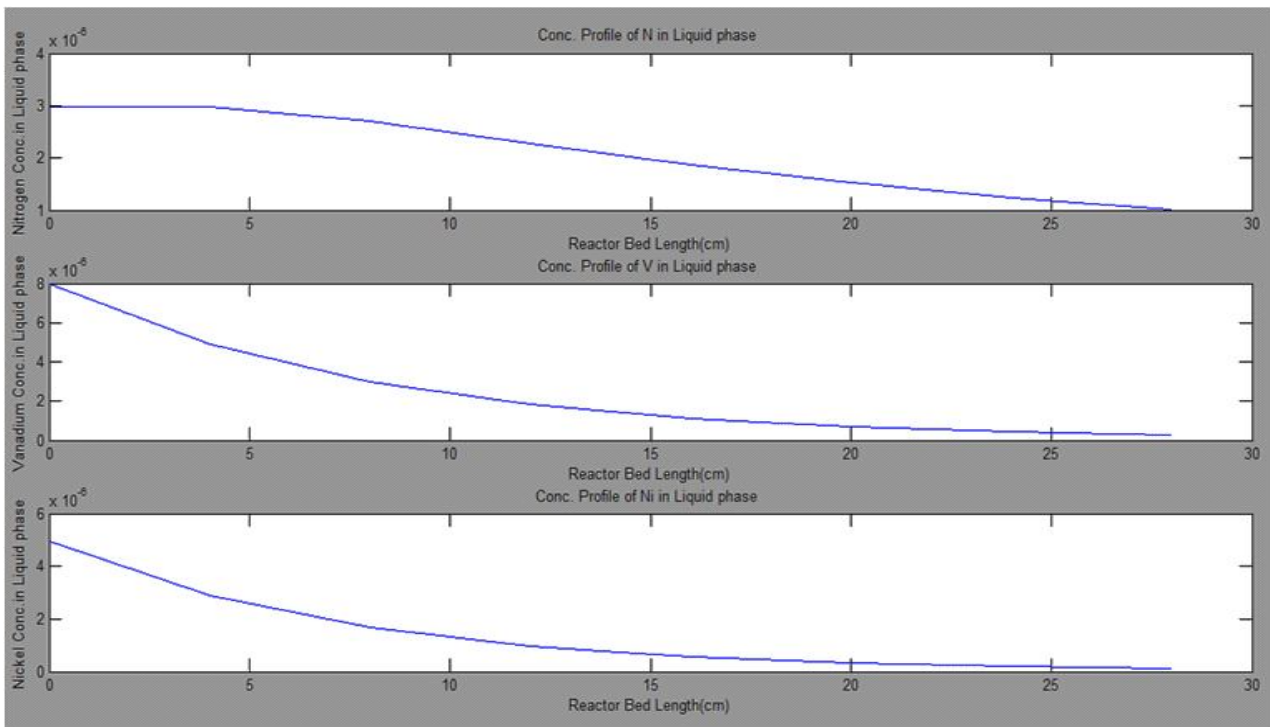


Figure 11 : Variation of N , V , Ni Concentration in liquid phase along reactor bed length

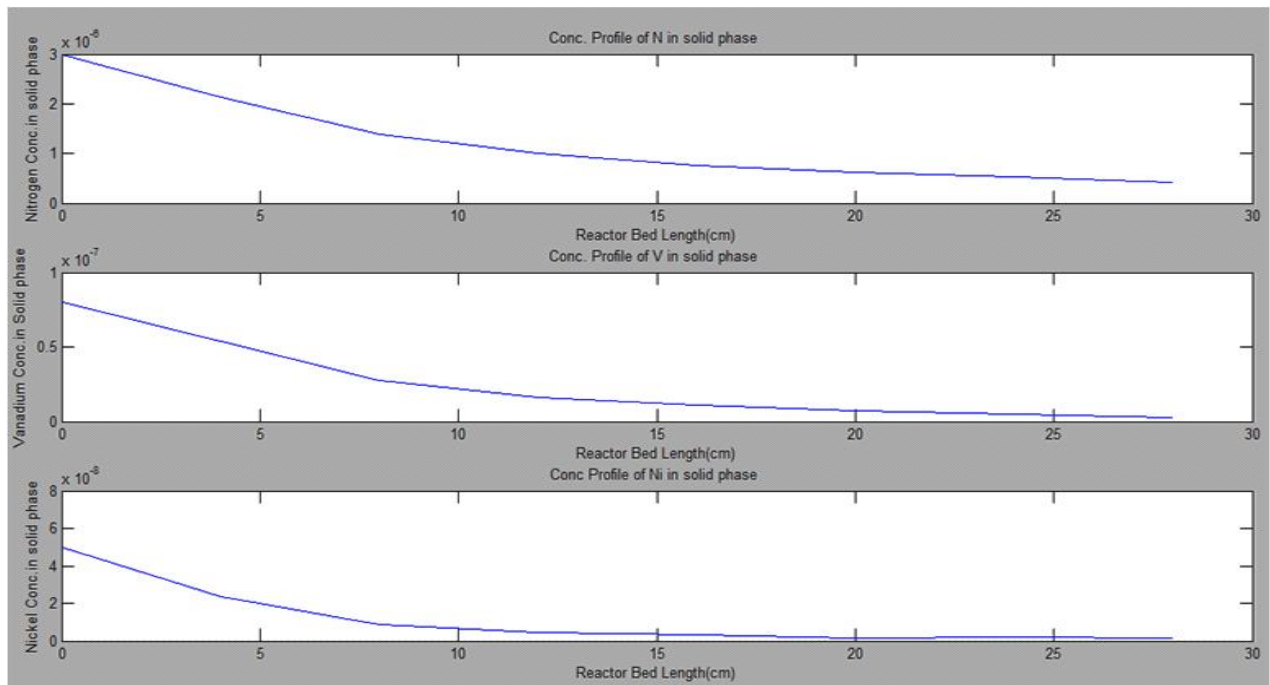


Figure 12: N , V , Ni Concentration in solid phase along reactor bed length

It is noticed that the hydrogen partial pressure in gas phase decreased along the catalyst bed length as a result of hydrogen consumption. Whereas, the concentration profile of hydrogen in the liquid phase and solid phase increased along the catalyst bed length. This behavior can be attributed to the difference in mass transfer rate at gas– liquid and liquid–solid, and reaction kinetics. When mass transfer at a liquid–solid interface becomes predominant, the H<sub>2</sub> concentration decreases in both the solid and liquid

phases, and when the mass transfer from liquid to gas becomes important, the liquid phase concentration also solid phase concentration increases.

The concentration profiles of N, V and Ni along the catalyst bed length in the liquid and solid phase can be seen from this figure, the concentration profile of these compounds reduced in both liquid phase and solid surface along the reactor bed length. In addition, there is a concentration gradient between both phases. This gradient is governed by liquid–solid mass transfer rate calculated from the equations used in this model, which is based mainly on the physical properties of the liquid, such as density and viscosity, and also liquid mass velocity. Therefore, the feedstock becomes lighter and thus physical properties are improved and mass transfer of liquid–solid will enhance reducing this concentration gradient

#### 4. Conclusions

The kinetic parameters estimations of trickle bed reactor mode for HDN, HDV and HDNi reactions of crude oil have been calculated using pilot plant experimental data and an optimization technique. The effect of reactor temperature (T), partial pressure of hydrogen (P) and liquid hourly space velocity (LHSV) upon the N, V and Ni conversion and upon the concentration profiles along the reactor bed length were studied using the process model. It has been observed that the influence of these operating conditions in HDN, HDV and HDNi of crude oil confirming that high temperature, pressure and low liquid hourly space velocity improve the nitrogen, vanadium and nickel conversion. The model can now be applied to reactor design, operation and control, as well as to predict the concentration profiles of any compound at any conditions. A comparison between experimental results and model prediction results for HDN, HDV and HDNi of crude oil were plotted and the model simulation showed good agreement with the experimental results obtained from literature.

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