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# Simulation of packed bed reactors for naphtha reforming unit

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## Abstract

The study focused on the performance evaluation of catalytic naphtha reforming unit via a packed bed reactors arranged in series. Three series arranged packed bed naphtha reforming reactors were developed and simulated using Aspen hysys software and steady state performance models of the packed bed naphtha reforming reactor were developed through the application of the principle of conservation of mass and energy to predict both the yields of theses reactors, their dimensions in terms of length, diameter, height, volume and temperature effects or progressions along the reactors' length respectively. Three main reaction paths were considered in this research study that include the conversion of naphthenes to aromatics, naphthenes to paraffins and hydrocracking of paraffins. The developed performance models yielded first order ordinary differential equations which were solved using Runge-Kutta fourth order ODE45 solver. The packed bed reactor operating conditions of temperature and pressure are between 4800C and 5200C and 2atm respectively with ninety percent (90%) conversion. The simulated reactor performance model for the three reactors yielded 29.7 $m^3$, 40.78 $m^3$ and 52.33 $m^3$ for reactor volume, catalyst bed height of 11m, 12.98 m, 16 m, and reactor's diameter of 1.85 m, 2 m and 2.04 m respectively.

**Keywords:** Series Reactor; Naphthenes; Aromatics; Paraffins; Simulation; Aspen Hysys

## 1 Introduction

The blending of Naphtha produced from the atmospheric distillation of crude oil with several intermediates obtained from complex refinery processes produces Gasoline. With the emergence of more stringent environmental laws and alternating market demands have affected refinery processes [1]. The use of internal combustion engines has made gasoline production the major refinery procedures as a result of the amounts of available gasoline obtained in distillation solely were less than the demands from customers [2] Hence, additional refining of other petroleum fractions such as cracking, reforming and alkylation have been engaged to keep up with the demand of more gasoline [3]. The characteristic constituents of gasoline hydrocarbons (in % volume) is: 4-8% alkanes; 2-5% alkenes; 25-40% isoalkanes; 3-7% cycloakanes; 1-4% cycloalkenes; and 20-50% total aromatics (0.5-2.5% benzene) enhancing stability and performance are achiever by introduction of additives and blending mixture [4]. They include anti-knock agents, antioxidants, metal deactivators, lead scavengers, antirust agents, anti-icing agents, upper-cylinder lubricants, detergents and dyes. Gasoline product gotten from the process normally has over 150 different compounds, even though at least a thousand compounds have been identified in some blends. Although gasoline is engaged only in internal combustion engines, it has varying chemical composition as a result of the type of crude refined, available refining process, overall product demand and specifications [5].

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As a result of stringent environmental laws, refineries have actively engaged reduction of aromatics in gasoline by formulation adapting. Several nations have decreased the overall aromatics percentage in gasoline to about 35 - 42 volume percent [6]. The emission of carbon monoxide (CO), lead oxide and other harmful substances from the exhaust pipe of the automobile engine have resulted into serious environmental challenges as the ignition, combustion and induction stroke of car engine reach appreciable combustion power. The worrisome problem of pollution resulting into global warming, green-house effect, depletion of the ozone layer, acid rain, dissertation, deforestation and other related vices have agenda serious challenges as to the ability of man in producing automobile fuel that would save our environment and our globe at large from catastrophe. The use of anti-knock property Tetra Ethyl Lead (TEL) is fast becoming unpopular despite its competent as a good octane booster to give room to an alternatively environment-friendly gasoline for optimal engine performance without the formal introduction of lead [2]. The Catalytic reforming unit transforms straight run naphtha of low octane rating from the atmospheric distillation unit of crude to reformate, which are used as blending stocks with gasoline produced from other units of the refinery. This is accomplished through the conversion of paraffins (linear alkane hydrocarbons) to isoparaffins (branched alkanes) and the partially dehydrogenation of cyclic naphthenes (cycloalkanes) to form higher octane rating aromatics occurring with a relatively small change in the boiling range as the molecular hydrocarbon structures are simply reorganized with minimal amount of cracking [3, 7, 8] . The Octane rating is a fundamental value of motor fuel and is the ability or resistance of a fuel to knocking in comparison to the antiknock quality of iso-octane, hence the greater the octane rating of a gasoline the higher the compression ratio the fuel can withstand before detonating [9]. The enhancement of the octane number is achieved by the formation of aromatic compounds through several reactions, such as dehydrogenation, isomerization, cyclization and hydro-cracking; producing by-products of hydrogen ($H_2$) and liquefied petroleum gas (LPG). The branched and aromatic hydrocarbons will likely not ignite prematurely in internal combustion engines thus decrease knocking drastically [10]. All of the reforming catalyst in general use today contains platinum supported on silica or silica-aluminium base. In many cases rhenium is combined as a second metal with platinum to form a more stable catalyst which permits operation at lower pressure. The presence of the second metal confers extra stability on the catalyst, thus slowing catalyst deactivation. The activity of this catalyst is further enhanced by fixing chlorine on the surface of the catalyst giving extra stability to the catalyst and this development has resulted in the new mechanical concept of the Universal Oil Product (UOP). Platinum serves as catalyst site for reactions of hydrogenation and dehydrogenation, whereas chlorinated alumina serves as an acid site for reactions of isomerization, cyclization and hydrocracking. Activity of reforming catalyst is dependent on surface area, pore volume and reduces while in operation by deposition of coke and loss of chlorine [11, 12]. The capability to sustain high catalyst activity by the process of continuous regeneration of the catalyst is the main pro of the continuous type unit. The benefit has to be assessed with respect to the greater costs of capital and likely lesser rates of hydrogen recycle and operating pressure required to maintain reduced coke level [13].

Therefore, this research study focused on modeling catalytic reforming unit as packed bed naphtha reforming reactor thereby evaluating the performance of the naphtha reforming unit through the development and simulation of naphtha reforming process using Aspen Hysys software, development of performance model equations for packed bed naphtha reactor via the application of the principle of conservation of mass and energy, simulation of the naphtha reforming process by solving the developed performance model equations and validation of the performance model with plant data.

## 2 Material and methods

The materials applied in this research study include packed bed naphtha reactor, series reactor, Aspen Hysys, plant data etc

### 2.1 Method

The following methods are applied in performing this research study.

#### *2.1.1 Process Description*

The reaction pressure is achieved by pumping of the liquid charge and the ensuing liquid-gas mix goes into a heat exchanging system for preheating. The temperature of the first reactor feed is raised and it completely vaporizes in the process as shown in Figure 1. As the reactants that are vaporized pass through the catalytic packed bed reactor, the main reaction is the formation of aromatics by dehydrogenation of naphthenes that is endothermic in nature thereby leading to temperature reduction between the reactor inlet and outlet. To sustain the necessary temperature for the reaction and the reaction rate, the vaporized stream is heated again in the fired heater prior to entering the second reactor. Also, there will be temperature drop in the second reactor, leading to temperature increase of the process via

the heater before transfer into the third reactor. As the operation progresses within the reactor, there is reduction in reaction rate as the volume of reactor increases.

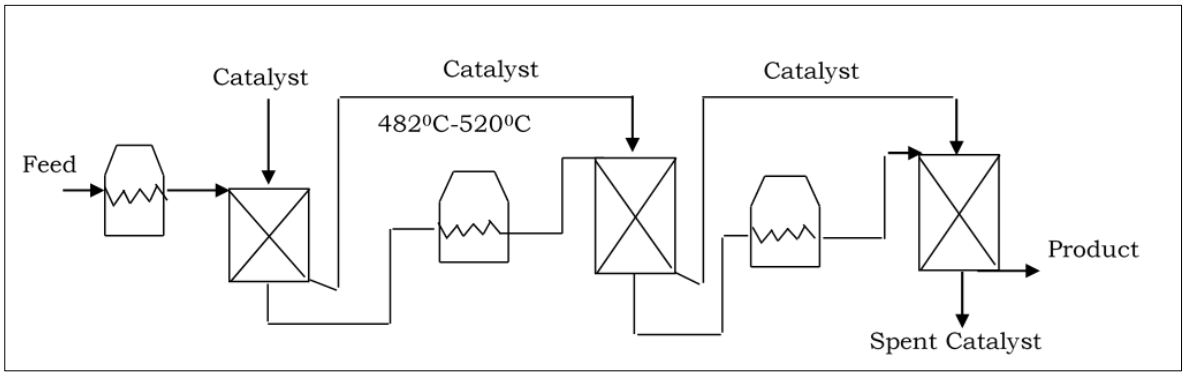



**Figure 1** Packed Bed Naphtha Reforming Reactor

Thus, upgrading the octane number of gasoline requires inter stage heat transfer in a series of reactors and the more compact the hydrocarbon molecule for a given number of carbon atom, the greater the octane number and hence, the necessity of turning straight-chained hydrocarbons to branched-chained isomer molecules. Furthermore, the described process analysis is designed using Aspen Hysys software as shown in Figure 2

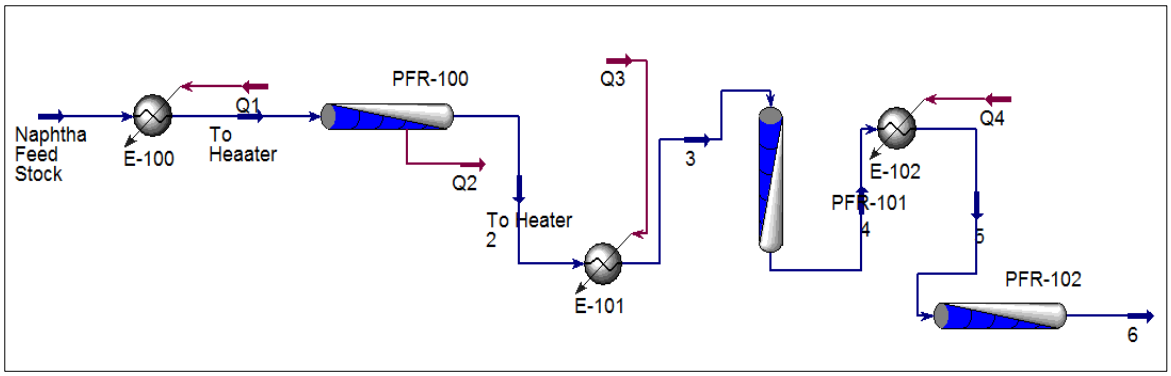
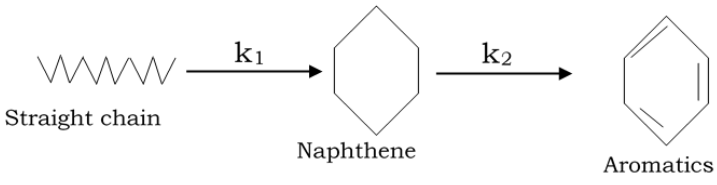



**Figure 2** Aspen Hysys Naphtha Reforming Process

*2.1.2 Kinetics of the Process*

A kinetic model is an essential tool for the adequate design and solution of chemical processes [14, 15]. The kinetics of the reaction therefore refers to the rate equation and rate constant of the reaction taking place in the process [16]. Naphtha is a very complex mixture of hydrocarbon and due to the large number of components involved in the reactions, the development of kinetic models becomes very complex [17]. Akpa and Adeloye states four categories of reactions that occur in the reactor which include transformation of naphthenes to aromatics, hydrogenation of naphthenes to paraffins, hydrocracking of paraffins and hydrocracking of naphthenes [3]. The stoichiometric equation of the reaction.




(1)

The first reaction step is slow compared to the second reaction step, and each step is highly endothermic. Hence, heat exchangers are installed at the inlet of each reactor to maintain the feed temperature to the reaction desired temperatures and above 500⁰C undesirable side reactions occur, while below 121⁰C, the reaction does not occur (no reaction takes place below this temperature)..

In Addition, Akpa and Adeloye expressed rate equations and rate constants for the reaction process thus [3].

- Naphthenes to Aromatics

$$r_1 = \eta\rho_b k_{P1}\left(P_N - \frac{P_A {P_N}^3}{k_{Pie}}\right) \quad (2)$$

$$k_{P1} = e^{\left(23.21 - \frac{34750}{1.8T}\right)} \quad (3)$$

$$k_{Pie} = e^{\left(46.15 - \frac{46045}{1.8T}\right)} \quad (4)$$

- Naphthenes to Paraffins

$$r_2 = \eta\rho_b k_{P2}\left(P_N P_H - \frac{P_N}{k_{P2e}}\right) \quad (5)$$

$$k_{P2} = e^{\left(35.98 - \frac{59600}{1.8T}\right)} \quad (6)$$

$$k_{P2e} = e^{\left(\frac{8000}{1.8T} - 7.12\right)} \quad (7)$$

- Hydrocraking of Paraffins

$$r_3 = \eta\rho_b k_{P3}\frac{P_p}{P_t} \quad (8)$$

$$k_{P4} = e^{\left(42.97 - \frac{62300}{1.8T}\right)} \quad (9)$$

The factor of catalyst efficiency is a measure of how much the feedstock reaction rate is lowered due to the resistance to pore diffusion through the catalyst [18]. Thus, the efficiency factor of reaction depicts the ratio of the rate of reaction into the particle to the particle surface reaction rate as posited by Mohammed *et al*. [19] and is evaluated as a Thiele Modulus function valid for cylindrical particle.

$$\eta_j = \frac{tanh\varphi_j}{\varphi_j} \quad (10)$$

### *2.1.3 Development of Performance Model Equations*

The performance model equations for catalytic naphtha reforming process are developed through the application of the principle of conservation of mass and energy based on these underlined assumptions.

- The components in the reactor moves in a plug flow manner such that concentration varies along the length of the reactor bed
- The reactor operates under steady state condition
- Reactions are in the same phase (homogenous reactions)

Material Balance Equation

The material balance equation was developed based on the principle of conservation of mass by considering a fixed packed bed reactor operating at steady state condition.

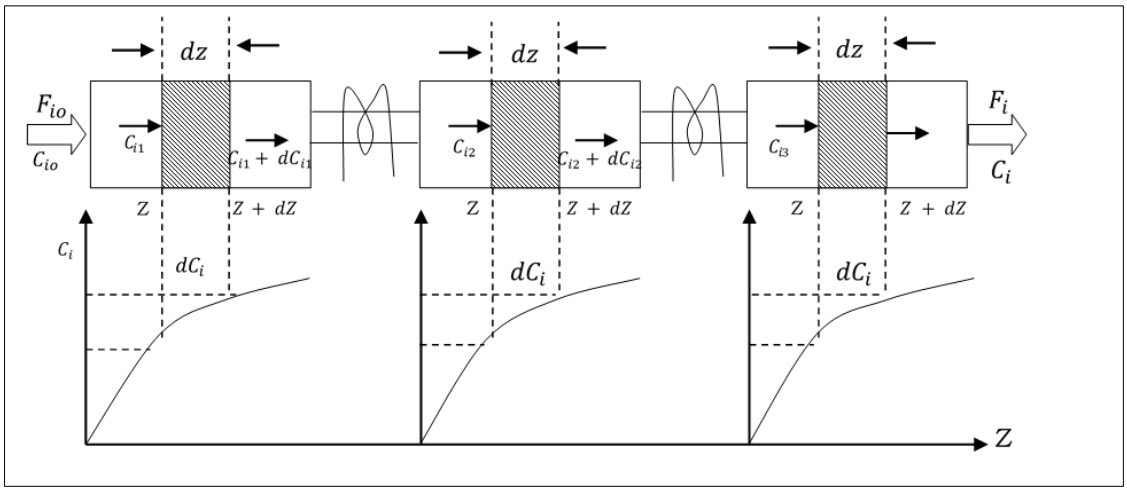



**Figure 3** Packed Bed Naphtha Reforming Reactor

By applying the principle of conservation of mass on the differential element of the packed bed of naphtha reactor gives:

$$[Rate\ of\ accumulation\ of\ component\ i] = [Rate\ of\ input\ of\ component\ i] - [Rate\ of\ output\ of\ component\ i] \pm [Rate\ of\ generation\ or\ depletion\ of\ species\ i] \quad (11)$$

Therefore, the volume of reactor can be determined from Equation (11)

$$\frac{V_0 dP_i}{RT} = (-r_i)d\mathrm{v} \quad (12)$$

Energy Balance Equation

Considering a tubular reactor in which heat is evolved or absorbed through the cylindrical walls of the reactor, and assuming no radial gradient in the reactor.

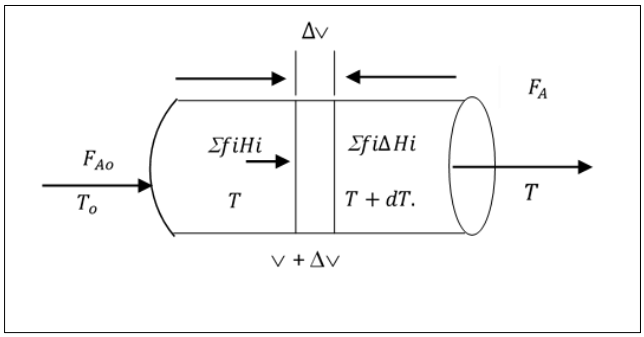



**Figure 4** Naphtha Packed Bed Reactor

The general energy balance equation over a differential element as shown in Figure 4 can be expressed thus.

$$[Rate\ of\ accumulation\ of\ energy\ by\ component\ i] = [Rate\ of\ input\ of\ energy\ by\ component\ i] - [Rate\ of\ output\ of\ energy\ in\ component\ i] \pm [Rate\ of\ generation\ or\ depletion\ of\ energy\ due\ to\ chemical\ reaction] \quad (13)$$

Therefore, the temperature variation in the reactor is expressed as

$$\frac{dT}{dW} = \frac{(\Delta H_e)(ri) - 4U/\rho_b D\,\Delta T}{\rho_b \sum C\rho i Fi} \quad (14)$$

Heat Load

The heat load is a function of molar flow feed rate, the degree of conversion and heat of reaction and is expressed as;

$$Q = \Delta H^{O}{}_{R}\left(\frac{P_{io}V_o}{RT}\right)\left(1-\frac{P_i}{P_{io}}\right) \quad (15)$$

Pressure Drop along Reactor Length

The pressure drop along the reactor length is one of the performance measures of a packed bed reactor.

$$\therefore \quad \Delta P = \frac{0.16L\ f^{\,0.84}\ \mu^{\,1.84}\ \mu^{0.16}}{D^{0.16}} \quad (16)$$

### 2.2 Solution Technique

The developed model equations for the packed bed reactor yielded a set of first order differential equation, which are solved numerically using the fourth order Runge-Kutta fourth order algorithm coupled in MatLab solver.

#### *2.2.1 Models Validation and Simulation*

The results of the developed model for the series packed bed reactor were validated with the Aspen Hysys result to test the suitability of the models in predicting the conversion or yield of the products

## 3 Results and discussion

The results of the developed model for catalytic naphtha reforming unit are discussed thus.

### 3.1 Reactors Dimension

The dimensions of the three reactors in terms of volume, length, diameter and void fractions are evaluated as shown in Table 1.

**Table 1** Dimension of the Three Reactors

| Functional parameters | Reactor 1 | Reactor 2 | Reactor 3 |
|---|---|---|---|
| Volume of reactor ($m^3$) | 29.7 | 40.78 | 52.33 |
| Length of reactor (m) | 11 | 12.98 | 16 |
| Diameter of reactor (m) | 1.85 | 2 | 2.04 |
| Void fraction of reactor | 0.6 | 0.6 | 0.6 |

### 3.2 Variation of Volume of the Reactors with Conversion

The volume of the reactor shows the total area and height occupied by the catalyst packed bed reactor, thus the capacity of the reactor as shown in Figure 5.

The volume of each reactor increases as the conversion also increase, depicting that the conversion is directly proportional to the volume of reactors. This increment was due to the fact that the reacting species had large surface area (catalyst bed) to reacts, this large surface area for reaction led to an increase in reaction operational rate and consequent improved product yield,.

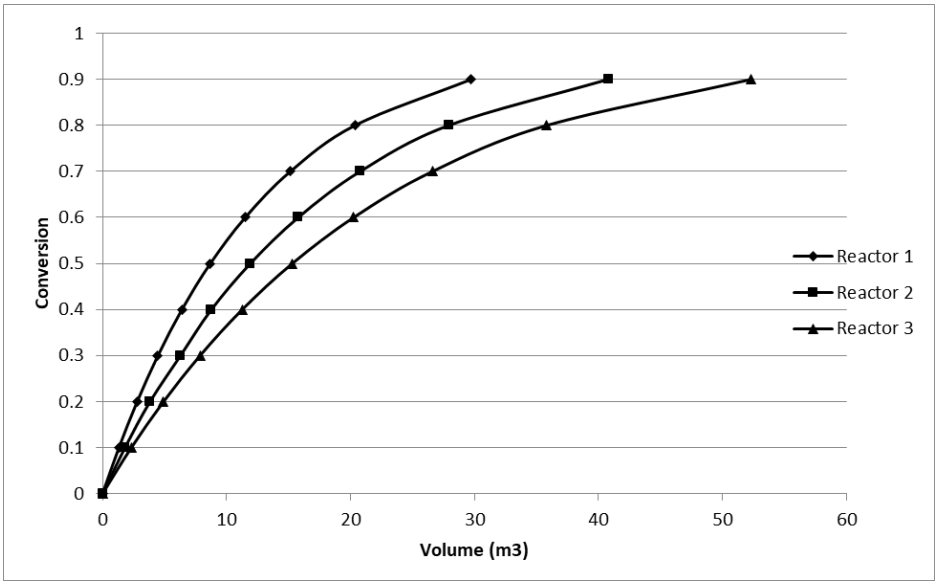



**Figure 5** Volume Variations with Conversion for the Three Reactors

### *3.2.1 Variation of Catalyst Bed Height with Conversion*

The Catalyst bed height of the reactor is an important functional parameter for reactor modeling, design and analysis, as it gives an idea on the height of the reactor. Figure 6 showed that as the catalyst bed height of the reactors increases, the reaction rate also increases due to the activity of the reactor catalyst.

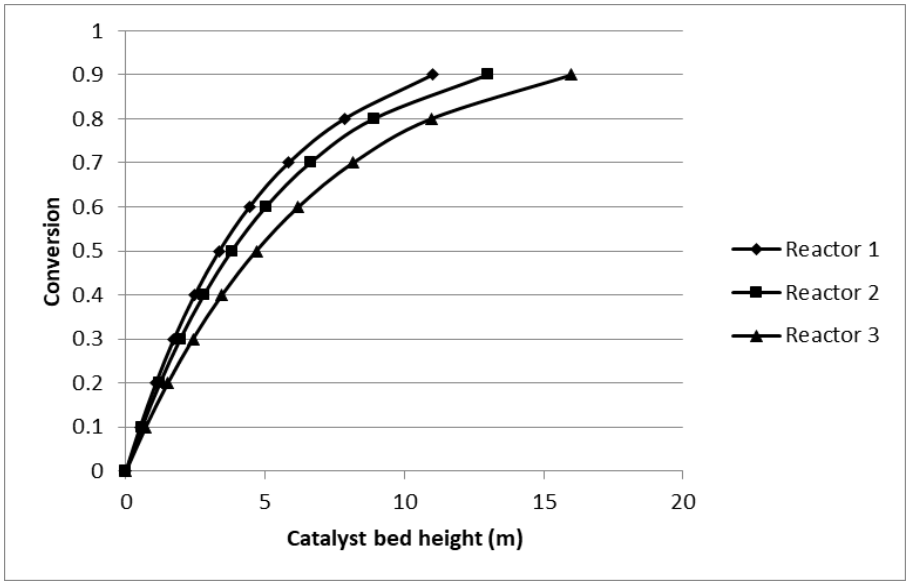



**Figure 6** Catalyst Bed Height with Conversions

Thus this increment was due to the fact that in packed bed reactors, the rate of formation of product increases along the catalyst bed height of the reactors due to a higher conversion rate which resulted to an increase in the yield of product.

## 3.3 Variation of Pressure Drop along Catalyst Bed height

The variation of pressure drop across the catalyst bed height showed a decline in value along the catalyst bed height as depicted in Figure 7. These decline in values were due to pressure drop along the catalyst bed height as the operational process progresses.

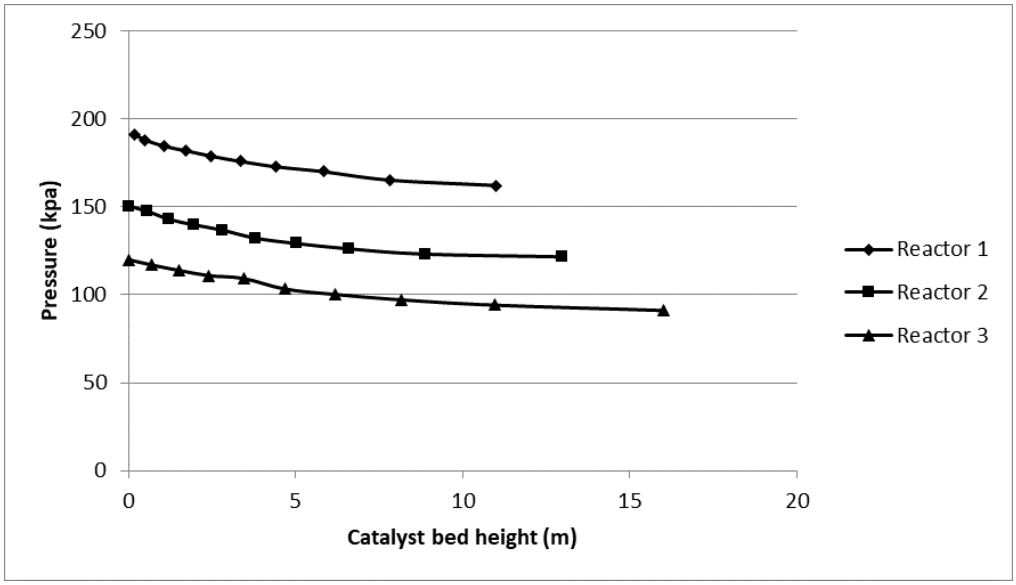



**Figure 7** Pressure Variations along Catalyst Bed Height

### 3.4 Heat Load

The heat load refers to the amount of heat required in maintaining the temperature of the reaction process.

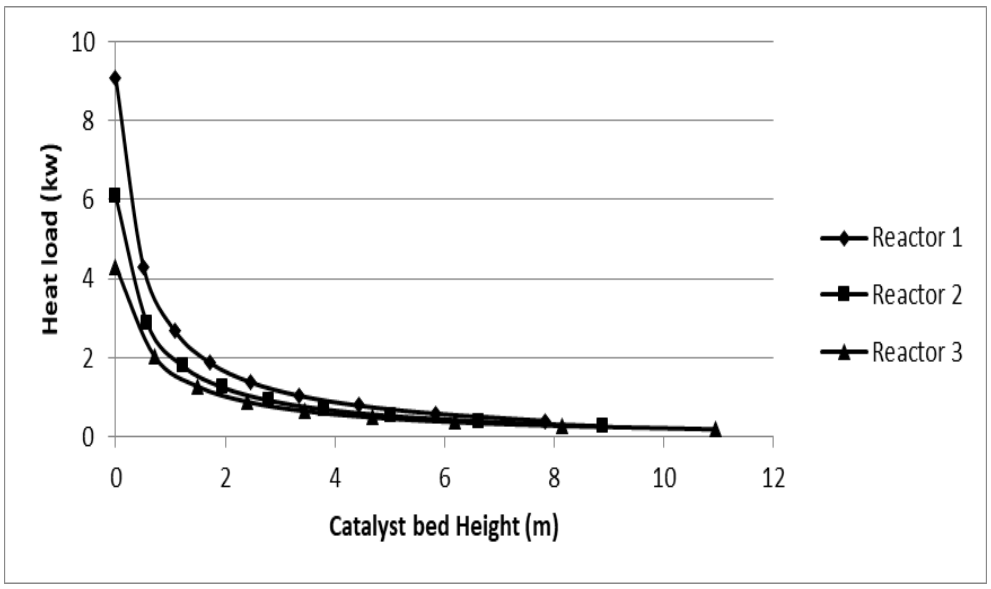



**Figure 8** Heat Load Variation along Catalyst Bed Height

It could be seen from Figure 8 that the heat load decreases along the catalyst bed height, the decrease is due to the endothermic nature of process.

### 3.5 Temperature Variation along the Catalyst Bed Height Reactors

Figure 9 shows temperature variation in reactor 1, thus there is a rapid decrease in the temperature along the catalyst bed height of the reactor 1. This decrease in temperature of the reactor along the catalyst bed height is due to the endothermic nature of the dehydrogenation reaction of naphthenic hydrocarbons to form aromatics.

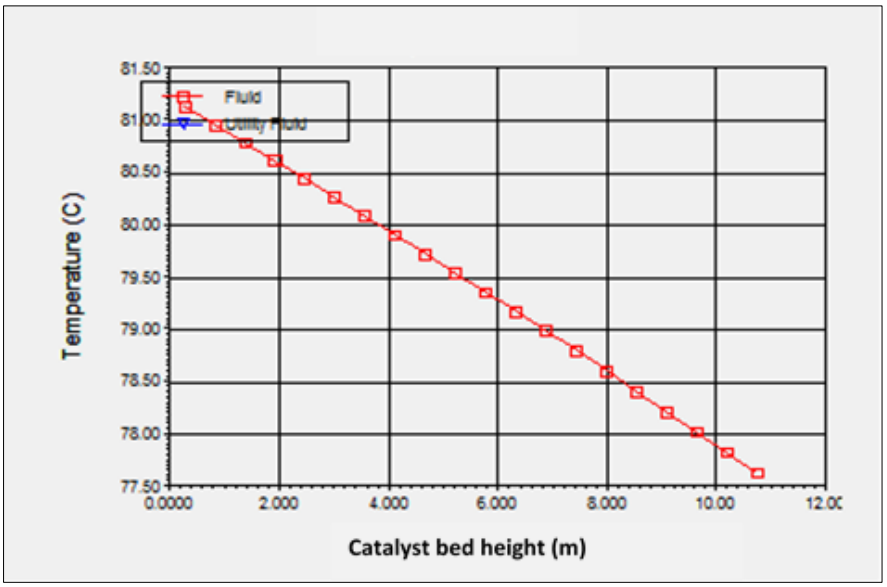



**Figure 9** Temperature Variation with Catalyst Bed Height

Also, Figure 10 showed that the reactor temperature in the second reactor decreases sparingly across the catalyst bed height due to the isomerization reaction.

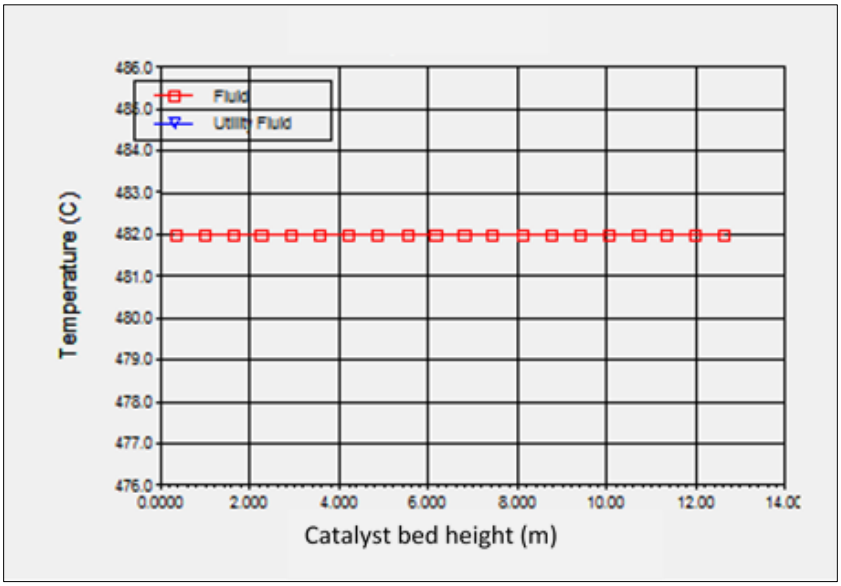



**Figure 10** Temperature Variations with Catalyst Bed Height

Therefore, the sparingly constant temperature was as a result of the thermo-neutral nature of the isomerization reaction that took place in the second reactor. In addition, Figure 11 depicted an exponential increase in temperature of the reactor along the catalyst bed height in reactor 3.

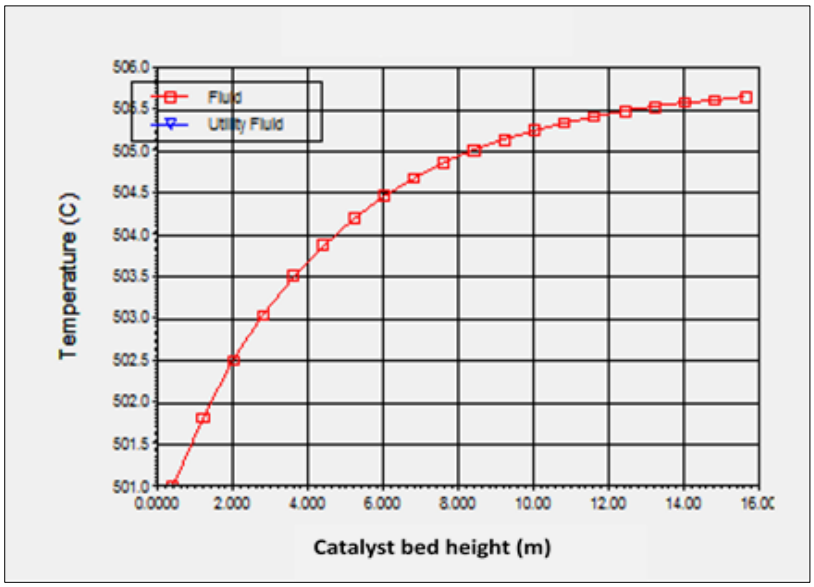



**Figure 11** Temperature Variations with Catalyst Bed Height

Hence, the temperature increase is due to the exothermic nature of the hydrocracking reaction occurring in reactor 3 for the formation of aromatics.

*Nomenclature*

- $\eta$ is the effectiveness factor defined as a measure of how far the reactant diffuses into the catalyst pellet before reaction.
- is catalyst bed density
- L is reactor length
- $f$ is friction factor
- U is fluid velocity
- D is reactor diameter
- $\mu$ is fluid viscosity
- $\rho$ is fluid density

## 4 Conclusion

The refinery naphtha reforming unit was developed and simulated using Aspen hysys software for enhancement or production of more valuable petroleum products from the refinery secondary recovery process unit. Steady state performance models were developed for the packed bed reactor using the principles of conservation of mass and energy respectively. The developed model equations which were first order differential equation were solved using Runge Kutta fourth order ODE45 solver and the performance of the naphtha reforming unit simulated. The results of the developed and solved model equations were compared with Aspen hysys results and the results comparison deviation or absolute error is minimal and within the allowable or acceptable value.

## Compliance with ethical standards

*Acknowledgments*

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*Disclosure of conflict of interest*

We the authors discloses that there is no conflict of interest in carrying out this research study.

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