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Optimization of Gasoline Product Yield from Riser Reactor Using Five Lump Kinetic Scheme

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Abstract: The research focused on vacuum gas oil consumption as feedstock to packed bed plug flow riser reactor of fluid catalytic cracker unit for optimized yield of gasoline, liquefied petroleum gas and fuel gas products and minimal yield of coke as undesired product. Therefore, steady state material and energy balance model equations were developed for packed bed plug flow riser reactor of fluid catalytic cracker using five lump kinetic schemes. These models were developed for the fluid catalytic cracking riser reactor as packed bed plug flow reactor using the principles of conservation of mass and energy balances respectively. The optimized gasoline yield of 56.47% was achieved in this research and when compared with refinery plant data and other previous research via a fluidized bed rise reactor model, showed a higher gasoline product yield. The optimized gasoline yield is also attributed to the efficacy of kinetic parameters (pre-exponential factors and activation energies) estimation. The developed material and energy balance ordinary differential model equations were solved using MatLab software and simulated results compared with refinery plant data with good alignment. The developed ordinary differential model equations simulated and yielded optimized gasoline yield of 56.47%, liquefied petroleum gas yield of 18.24%, flue gas yield of 15.49% and coke yield of 3.16%.

Keywords: Riser Reactor, Lumping Scheme, Modeling, Simulation, Gasoline Yield.

Research Paper

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1.0 INTRODUCTION

Fluid catalytic cracking (FCC) as a significant refining process is the core operation for the transformation of heavier feedstock to less heavy, more important products like LPG (Liquefied Petroleum Gas) and naphtha that is cracked, the main components of the gasoline loch (Dagde, 2018). Also, per the preferred cracking reactions, development of coke transpires in these processes (Shayegh *et al.,* 2012). While the coke is in the regenerator, it is transformed to CO, CO_2, H_2O, SOx, and NOx compounds (Gauthier *et al.,* 2000). Also, fluid catalytic cracking has become undoubtedly an apex in petroleum refinery: applied in the conversion of vacuum residues, straight-run atmospheric gas oil, besides further relatable heavy stocks to a large broadband of outputs using a catalyst (Akah, 2017). The products of catalytic cracking are mainly fuel gas, great octane gasoline, liquefied petroleum gas, diesel fuel, light fuel oil, heavy fuel oil etc. (Dagde & Puyate, 2012). The major conversion processes in an integrated refinery complex remains a vital responsibility of fluid catalytic cracking (FCC), and catalytic cracker remains the password to profitability for many refiners (Ahmed *et al.,* 2014). Majority of the FCC units in existence have been improved by six major technology licensers from which the universal oil products (UOP) presently owned subordinate of Honeywell is the mostly used (Sildir *et al.*, 2015). FCC unit is mostly introduced to transfigure the high-molecular weight, high-boiling hydrocarbon crude oils segments to further appreciated olefinic gases, gasoline and other products (Amino *et al.*, 2012). Thermal cracking can also be used to crack petroleum hydrocarbons, but several research works has shown that the use of FCC to crack petroleum hydrocarbon is preferred to that of thermal cracking since it in addition, produces gaseous by-products that have additional C=C bonds (added olefins), therefore, economically added valuable instead of cracking thermally (David & Peter, 2006). Upon heating, feed is met with a high-temperature catalysts in powered form, this unlinks the long-chained bonds of the high temperature boiling liquid hydrocarbon into much short-chained bonds and are collected as vapour (Debasis, 2011). Current units have been redesigned to channel heat from the regenerator as a means to the required amount of heat for the riser reactor and also heat the feed up to reaction temperature (Fernandes *et al.*, 2007). Various researches have been carried out for FCC modeling, simulation, optimization and control, yet only a hand-full (few) of them put into cognizance, the RFCC (Xu *et al.,* 2006). Souzaa *et al.*

(2003) used a 2-Dimensional fluid flow field having a 6-lump Kinetic model also having two energy balance models (gas oil and catalyst) to describe the process of cracking of the gas oil in the riser reactor. Das *et al.,* (2003) conducted 3-D simulation of a large-scale FCC riser reactor. Berry *et al.,* (2004) modify and improved the 2-D hydro-dynamic model to enable it predict by including the slip factor for the determination of the cross-sectional average voidage.

There are some other useful models like, the Hydro-dynamic model of (McCabe & Smith, 2004) which is improved by (Bhende & Patil, 2014). To solve for the riser operating conditions in an industrial FCC units. Salts still entrained serve as a basis of metals that can poison costly catalysts employed in several crude refining complex processes (Wauquier, 2000). The droplets of water coagulates and settles to the depth of the tank (Pereira *et al.,* 2015). Hydro-desulfurized products are treated and mixed or employed as feed for catalytic reformer (Cheremisinoff & Rosenfeld, 2010). The fluid catalytic cracking unit is a complex unit and of great economics importance in producing high octane value gasoline, thereby providing reasons for extensive research in the process of developing models, simulation and optimization of products yield of the fluid catalytic cracker riser reactor. Thus, the fluid catalytic cracking unit is an integral unit of conventional major refineries worldwide as it accounts for over sixty percent (60%) of valuable products such as LPGs, gasoline, fuel gas, as well as coke. Hence, the necessity for the development of appropriate model equations for the fluid catalytic cracking riser reactor to optimize its main products yield. Therefore, this research focus on optimization of gasoline product yield from the riser reactor unit of fluid catalytic cracker by defining appropriate kinetic rate equations using the lumping scheme, application of the principle of conservation of mass ad energy balance to develop material balance expression that will predict the riser reactor products yield and the riser reactor exit temperature respectively, analysis of the riser kinetic parameters, simulation of the developed model equations using industrial plant data and optimization of the product yield through parametric study.

2.0 METHODS

2.1 Development of Riser Reactor Rate Equation

The fluid catalytic cracker is in two zones, riser and regenerator reactors but the cracking operations or processes occur in the riser reactor of the fluid catalytic cracking unit. Hence, the riser cracking operation in this research applies five reaction pathways as shown in Figure 1.

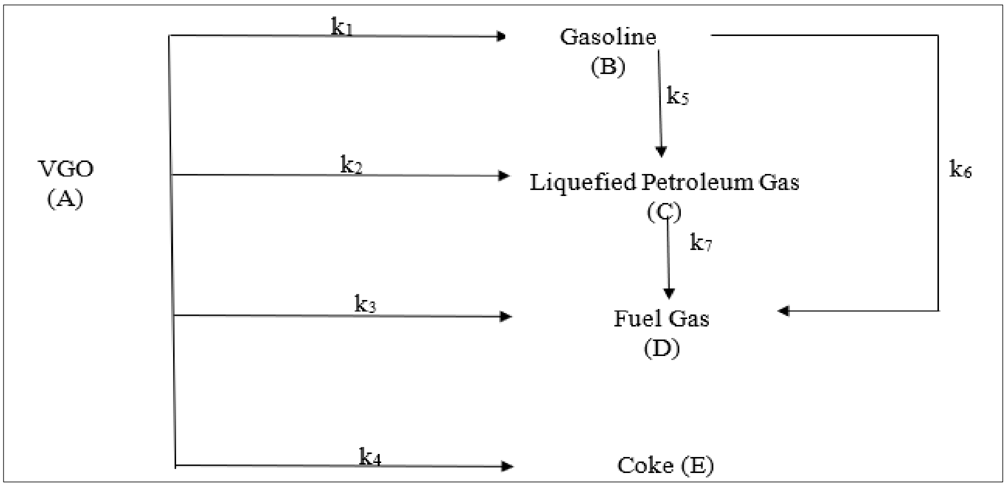

Figure 1: Pathway for Five Lump Process

The rate of reaction for each component is described based on mass fraction and the diffusion effect of gas-oil via the catalyst pore network using effectiveness factor. Writing the reaction rate equations in standard form yields

a. Gas Oil (A)

$(-r_A) = (k_1 + k_2 + k_3 + k_4)\, y_A^2 Ø\eta$ (1)

b. Gasoline (B)

$(-r_B) = [(k_5 + k_6)\, y_B - k_1 y_A^2]\, Ø\eta$ (2)

c. Liquefied Petroleum Gas (C)

$-r_c = (k_7 y_c - k_2\, y_A^2 - k_5\, y_B) Ø\eta$ (3)

d. Fuel Gas (D)

$-r_D = -(k_3 y_A^2 + k_6 y_B + k_7\, y_c\,) Ø\eta$ (4)

e. Coke (E)

$-r_E = -k_4\, y_A^2\, Ø\eta$ (5)

Development of Material Balance Equation

Riser and regenerator reactors are the two main components of the fluid catalytic cracking unit, but the riser reactor is the main focus of this research as cracking processes takes place in this reactor. Hence, the riser reactor is modelled as a plug flow reactor. In the fluid catalytic cracking plant, every fuel formation involving cracking takes place inside the riser reactor. This makes the riser reactor possibly the most significant in the fluid catalytic cracking plant. Hence, a mathematical model is required in modifying and design changes in operation that enhances optimized yields from the process. Within

2 to 5 seconds, every reaction takes place inside the riser, resulting from the presence of efficient feed injection system inside the fluid catalytic cracking units. This is the main reason many available models in the literature analysed the riser with mass and energy balances of single dimension (Ahari *et al*., 2008; Li & Lu, 2016).

2.2.1 Riser Reactor Model Assumptions

The following assumptions were applied in modeling the fluid catalytic cracker riser reactor:

i. Constant heat transfer at the riser wall and the coke and the catalyst have the same specific heat
ii. At the riser inlet, there is instantaneous vaporization and uniform catalyst gas temperature in all parts of the riser.
iii. Movement of fluid is not hindered by deposits of coke on the catalyst surface. Plug flow of single-dimensional transport takes place in the riser devoid of axial and radial depression.
iv. Heat capacities and feed viscosity of all component are the same. In the catalyst particles, adsorption and dispersion are insignificantly minimal.
v. Changes in pressure through the length of the riser and the dynamics of the riser is very fast to ensure a quasi-steady state model. This is made possible by the static catalyst head inside the riser
vi. A steady state operation in the fluid catalytic cracker packed bed plug flow riser reactor

2.2.2 Material Balance Equation

The principle of conservation of mass was applied in the development of the material balance equation for the fluid catalytic cracker plug flow riser reactor as shown in Figure 2.

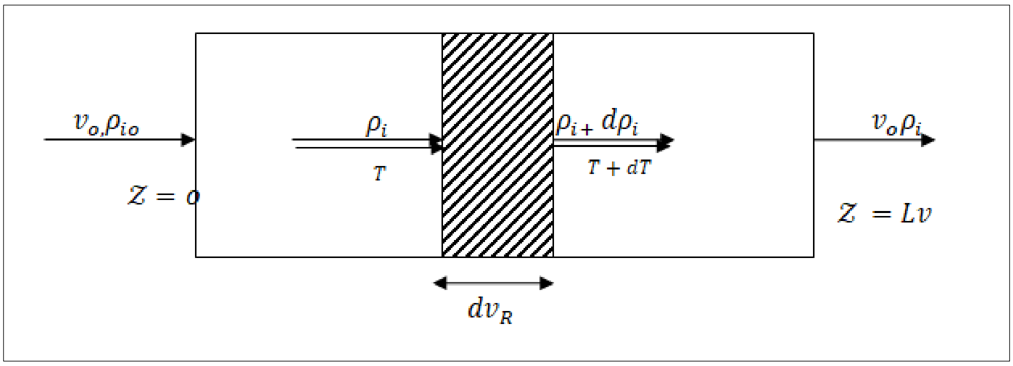

Figure 2: Packed Bed Plug Flow Riser Reactor

The material balance equation is expressed therefore as:

	Accumulation rate of mass of component *i* in the differential element	=	Inflow Rate of mass of component *i* into the differential element	
-	Outflow rate of mass of component *i* in the differential element	-	Disappearance Rate of mass of component *i* in the differential element due to chemical reaction	(6)

By the application of the model assumptions, mathematical analysis and upon variable separation of Equation 6 yields

$$-\frac{dy_i}{dZ} = (-r_i)\frac{\varepsilon_R L_v \rho_{gR} A_R}{F_{gR}} \quad (7)$$

Equation 7 is the steady state packed bed plug flow fluid catalytic cracking riser reactor.

Describing Equation 7 for each specie of the five lump scheme gives

i. Gas Oil

$$-\frac{dy_A}{dZ} = \frac{\varepsilon_R L_v \rho_{gR} A_R}{F_{gR}}(k_1 + k_2 + k_3 + k_4)\, y_A^2\, \emptyset\eta \quad (8)$$

ii. Gasoline

$$-\frac{dy_B}{dZ} = \frac{\varepsilon_R L_v \rho_{gR} A_R}{F_{gR}}[(k_5 + k_6)y_B - k_1 y_A^2]\, \emptyset\eta \quad (9)$$

iii. Liquefied Petroleum Gas

$$-\frac{dy_C}{dZ} = \frac{\varepsilon_R L_v \rho_{gR} A_R}{F_{gR}}[k_7 y_c - k_2 y_A^2 - k_5 y_B]\emptyset\eta \quad (10)$$

iv. Fuel Gas

$$-\frac{dy_D}{dZ} = \frac{\varepsilon_R L_v \rho_{gR} A_R}{F_{gR}}(-[k_3 y_A^2 + k_6 y_B + k_7 y_C]\, \emptyset\eta \quad (11)$$

v. Coke

$$-\frac{dy_E}{dZ} = \frac{\varepsilon_R L_v \rho_{gR} A_R}{F_{gR}}(-k_4 y_A^2\, \emptyset\eta) \quad (12)$$

2.2.3 Riser Reactor Energy Balance Equation

Along the length of the fluid catalytic cracker packed bed riser reactor, temperature distribution can be studied by applying the principle of conservation of energy on a differential element of the reactor shown in Figure 2. The principle of conservation of energy is expressed as:

	Accumulation Rate of heat in the differential element	=	Inflow Rate of heat into the differential elements	-	Outflow Rate of heat from the differential element	
-	Rate of heat generated within the differential element due to chemical reaction	(13)				

Upon substitution of terms, mathematical analysis and variable separation of Equation 13 yields

$$\frac{dT_d}{dZ} = -\frac{(\propto y_A^2 + \beta\, y_B + \gamma y_C)\, \emptyset \psi \rho_{gR}\, A_R\, \varepsilon_R\, L_v}{\left[F_{gR} C_{p_{gR}} + F_{cat}\, C_{p_{cat}}\right] T_{ref}} \quad (14)$$

Equation 14 is the general dimensionless steady state energy equation for he packed bed plug flow catalytic cracker riser reactor.

2.2.4 Riser Reactor Kinetic Parameters Estimation

The reaction rate constants, activation energies, pre-exponential factors etc. are important parameters to be determined and applied in simulating the packed bed riser reactor at steady state operations. This research applied kinetic parameters estimation method as evaluated by *Obi et al*., 2022 and Cyrus & Igbagara, 2025 in which regression analysis and MatLab were applied in solving complex and non-linear equations.

3.0 RESULTS AND DISCUSSION

3.1 Fluid Catalytic Cracking Riser Reactor

In validating the developed models for gas oil consumption and products yield for the five-lump riser reactor, the simulated results of the developed model equations are shown in Table 1 with its comparison with refinery plant data.

Table 1: Plant and Model Yields

Parameters	Plant Yield (%)	Model Yield (%)	Deviation
Gas Oil	26.6	6.6	0.752
Gasoline	45.9	56.5	0.231
Liquefied Petroleum Gas	17.0	18.2	0.071
Fuel Gas	5.4	15.5	1.870
Coke	5.1	3.2	0.373

The developed model yields higher or optimized gasoline, LPG, fuel gas products and reduced coke production with higher gas oil conversion when compared with plant data. Thus, the higher products yield is due to the efficiency of technique applied in deducing the process kinetic parameters in simulating the model equations.

3.2 Variation of Gas Oil and Products Yields

The results obtained from the developed models for the consumption of gas oil and products yield along reactor dimensionless length is depicted in Figure 3.

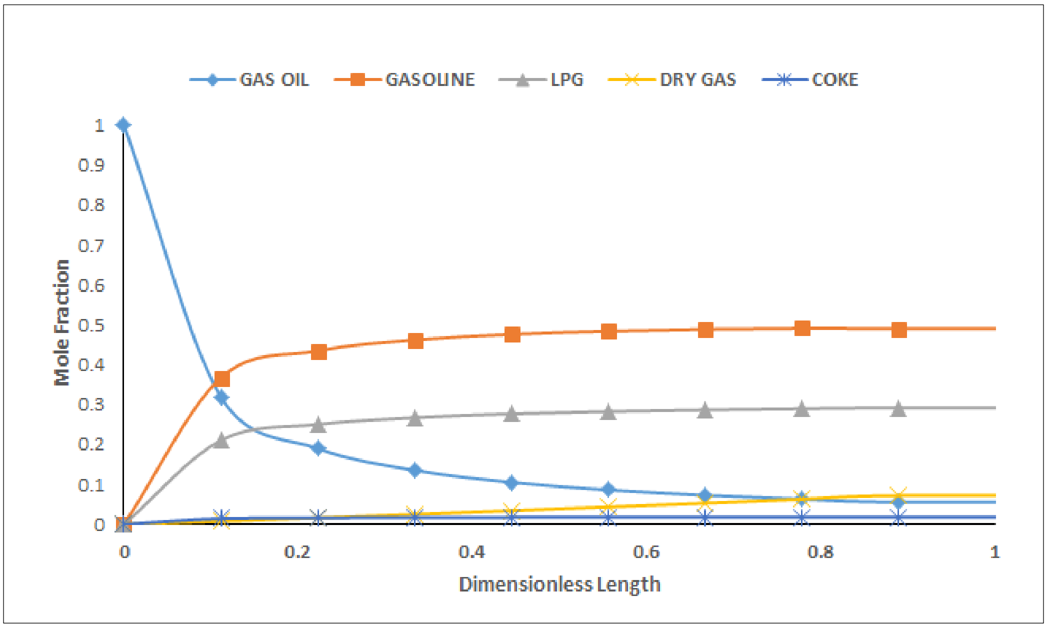

Figure 3: Variation of Gas Oil and Products Yield along Riser Reactor Length

The mass fraction of gas oil declines along reactor dimensionless length due to its consumption to lighter valuable products of gasoline, LPG, fuel gas and coke. Therefore, gasoline product yield increases to maximum while there is progressive yield of other products along the reactor dimensionless length and this is in tandem with the principle of chemical reaction engineering in which reactants are converted to products.

3.3 Effects of Products Yield with Gas Oil Conversion

The effects of vacuum gas oil conversion on gasoline, liquefied petroleum gas, fuel gas and coke yield are shown thus.

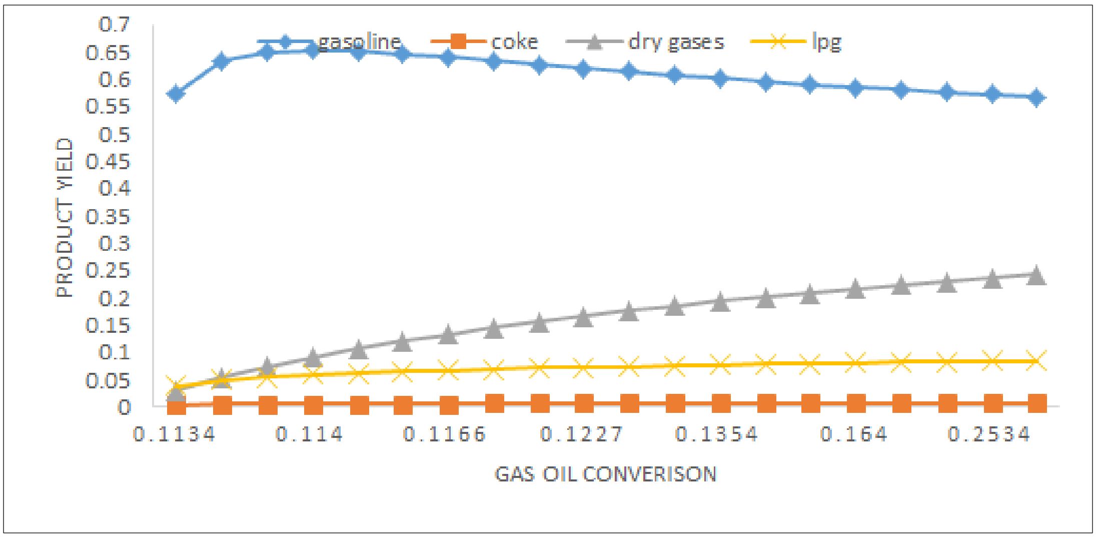

Figure 4: Effect of Products Yield with Gas Oil Conversion

Gasoline yield increases initially with vacuum gas oil conversion and approaches to maximum and there is steady reduction as a result of gasoline further cracking by acting as feedstock to yield other products such as liquefied petroleum gas and fuel gas respectively at high temperature range. Also, liquefied petroleum gas and fuel gas yields increase slightly as gas oil is converted and there is rapid increase in these products yield due to gasoline secondary cracking, while the yield of coke increase linearly as gas oil is converted. These results are due to vigorous mixing that ensures a constant reactor temperature is maintained as against decline temperature progression for the riser reactor. Therefore, a constant temperature throughout the bed favours the yield of liquefied petroleum gas, fuel gas and coke while higher yield of desired main product (gasoline) is obtained at lower reactor height.

3.4 Temperature Effects on Products Yield

The effects of temperature on products (gasoline, liquefied petroleum gas, fuel gas and coke) yield are highlighted in Figure 5.

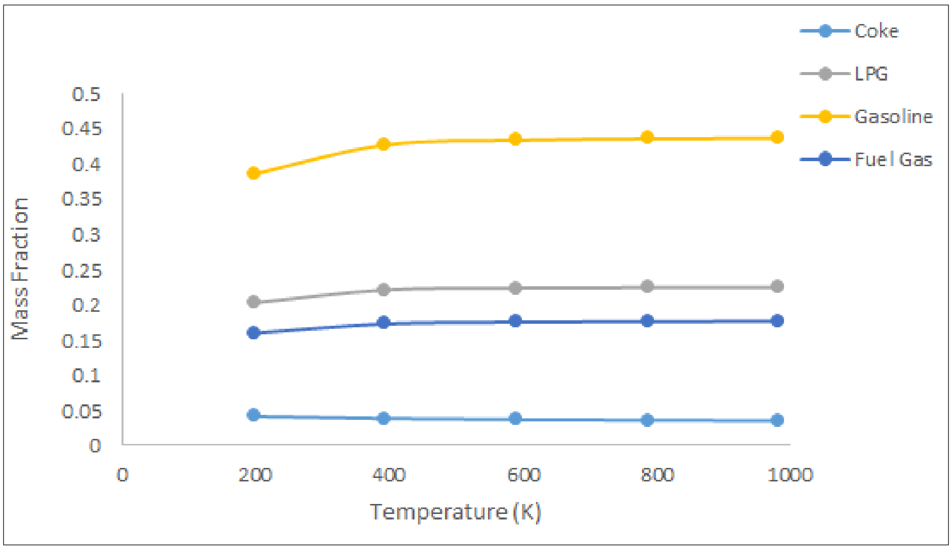

Figure 5: Temperature Effects on Products Yield

As temperature increases, the endothermic reaction of cracking vacuum gas oil to gasoline is enhanced with a linear progression curve but at higher temperature, gasoline secondary decomposition occurred to yield liquefied petroleum gas and fuel gas. The liquefied petroleum gas and fuel gas yield showed a gradual increase and at higher temperature, there is also a slight increase in their mass fraction as a result of gasoline decomposition. Hence, the temperature progression along the packed bed plug flow riser reactor is shown in Figure 6 and the progressive temperature decrease is due to the endothermic cracking reaction of gas oil to valuable products.

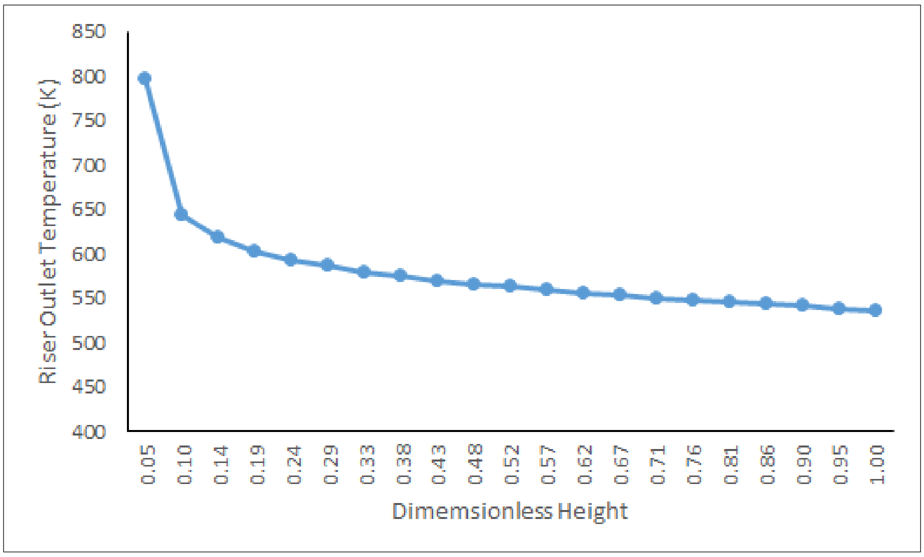

Figure 6: Temperature Progression along Reactor Dimensionless Length

3.5 Products Yield Effects with Mass Flow Rate of Gas Oil

The variation of vacuum gas oil mass flow rate varies directly with its velocity and inversely to gas oil residence time, hence increase in mass flow rates of gas oil increases its velocity with a decrease in vacuum gas oil residence time and a consequence decrease in cracking operation. This will lead to a decline in the conversion of gas oil and subsequent decrease in products yield.

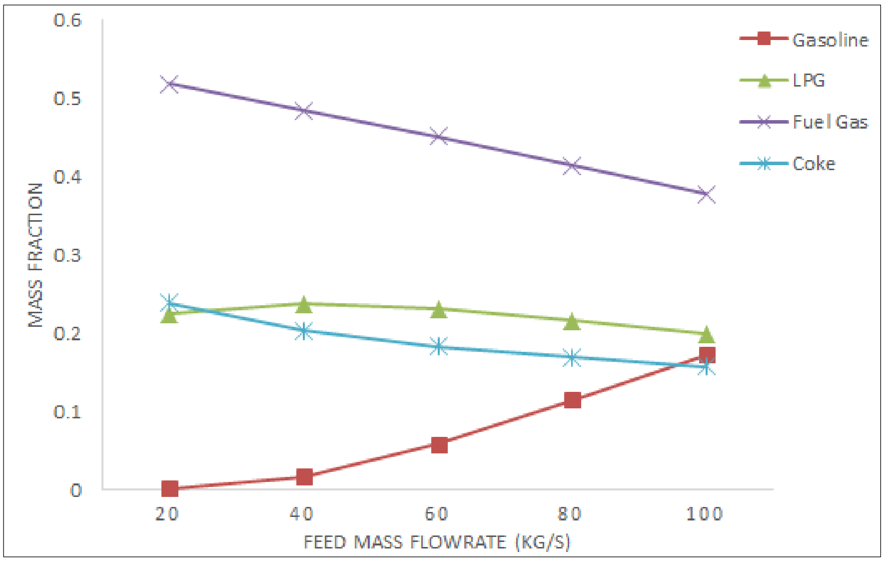

Figure 7: Products Yield against Mass Flow Rate of Gas Oil

There is general decline or reduction in liquefied petroleum gas, fuel gas and coke yield as the feed mass flow rate increases with a steady increase in gasoline yield based on the operational control. Also, increase in vacuum gas oil mass flow rate leads to increase in the inflow sensible heat associated with gas oil as shown in Figure 8.

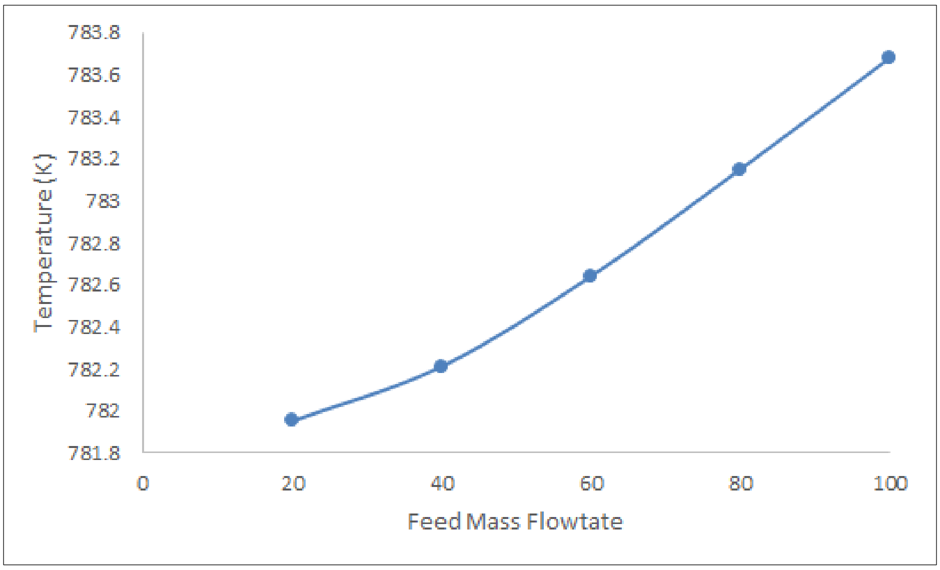

Figure 8: Riser Temperature with Mass Flow Rate of Gas Oil

Since increase in mass flow rate of vacuum gas oil results in decline of cracking process and reduction in the absorbed heat, the overall effects is higher riser outlet temperature.

4.0 CONCLUSION

The research focused on optimal yield of gasoline product via the modeling and simulation of packed bed plug flow riser reactor of fluid catalytic cracker using a five lump kinetic pathway. The research focused on improvement of the constraint of other previous studies, thus enhancing gasoline yield. The five lump kinetic rate equations were evaluated based on the reaction paths, thereby accounting for the riser reactor rate equations. Ordinary differential model equations were developed for the packed bed plug flow riser reactor using the five-lump pathway via the application of the principle of conservation of mass balance to predict vacuum gas oil consumption and products yield at steady state operation. Also, through the application of the principle of conservation of energy balance, a differential model equation was developed to predict exit temperature of the packed bed plug flow riser reactor at steady state process. Kinetic parameters of the five-lump rate equations such as pre-exponential constants and activation energies were applied based on the research of Obi *et al.,* 2022 and Cyrus & Igbagara, 2025 models. In addition, optimized gasoline product yield was achieved based on the research approach as he developed material balance equation was simulated and the process products yield were compared with refinery or industrial plant data. Hence, steady state developed model equations for the packed bed plug flow riser reactor of fluid catalytic cracker yielded an optimized gasoline product yield with minimal coke product yield due to efficient process kinetic parameters applied in simulating the packed bed plug flow riser reactor.

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NOMENCLATURES
- $k_1, k_2, k_3, k_4, k_5, k_6$ and k_7 are the intrinsic rate constants.
- ϕ is catalyst deactivation constant
- η is catalyst effectiveness factor
- r_A, r_B, r_C, r_D and r_E are the reaction rate of gasoil, gasoline, liquefied petroleum gas, fuel gas and coke respectively
- y_A, y_B, y_C, y_D and y_E are mass fraction of gasoil, gasoline, liquefied petroleum gas, fuel gas and coke respectively.
- y_{Ab0} *and* y_{Ae0} denotes gas oil inlet mass fractions both bubble/emulsion phase respectively y_{ib0} *and* y_{ie0} denotes inlet mass fractions of the products in both bubble and emulsion phases respectively.