

Transient Modeling and Simulation of Fluid Catalytic Cracker Riser Reactor

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Abstract: The research focused on conversion of vacuum gas oil to products via fluid catalytic cracker riser reactor and its transient performance or variation with parametric factors through the development of unsteady state or transient state partial differential model equations based on the principle of conservation of mass and energy balances. The transient state model equations were developed for fluid catalytic cracker riser reactor using five lump scheme to study vacuum gas oil feedstock depletion and (gasoline, liquefied petroleum gas, fuel gas and coke) yields. The developed plug flow partial differential equations for the fluid catalytic cracking riser reactor were solved using MatLab solver and simulated with industrial plant and literature data. The simulated results showed good accuracy with minimum deviation from industrial plant data due to the accuracy of kinetic parameters (activation energies, pre-exponential constants) data applied in solving and simulating the partial differential model equations. Therefore, the fluid catalytic cracker riser reactor performance was studied based on its feedstock and products yield variations with riser reactor dimensionless length and time, and its temperature variation along the riser reactor's length.

Keywords: Unsteady State Modeling, Plug Flow, Kinetic Parameters, Five Lump Scheme, Matlab

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 pool (Dagde, 2018). The catalyst in the FCC continuously goes through the FCC reactor (riser) plus the vessel regenerator. While the coke is in the regenerator, it is transformed to CO, CO₂, H₂O, SO_x, and NO_x compounds (Cerqueira *et al.*, 2008). 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 relating heavy stocks to a large broadband of outputs using a catalyst (Ahsan, 2015). 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). Refineries are characteristically large, sprawling industrial facilities with thorough piping present all over, transporting streams of liquids and gases between various chemical processing units (Sildir *et al.*, 2015). The major conversion processes in an integrated refinery complex remain a vital responsibility of fluid catalytic cracking (FCC), and catalytic cracking remains the passport to profitability for many refiners (Ahmed *et al.*, 2014). The FCC unit is mostly introduced to transfigure the high-molecular weight, high-boiling hydrocarbon crude oil 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 have 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). The feedstock into the FCCU is usually known as heavy gas oil (HGO) or also known as heavy vacuum gas oil (HVGO). (Debasis, 2011).

The reactor and regenerator material and energy balance are not simple (Ahmed & Ateya, 2016). Furthermore, it involves a compound hydro-dynamics and a great vagueness in the kinetics of the cracking reaction and the weakening of catalysts via deposition of coke (Cyrus & Igbagara, 2025). The transient modeling and prediction of catalytic crackers was studied and authenticated by comparing the general performance of the process with those in other research works was projected to be as an efficient instrument for numerous process system researches on the FCC processes (Saha & Dewangan, 2015). The most significant and commonly employed refining processes for producing more valuable gasoline by converting heavy oils and less heavy products by the catalytic cracking process. This causes the formation of coke (carbon). The carbon formed logs on the pore of the catalysts and progressively decreases the catalyst activity (Gauthier *et al.*, 2000). 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). Fluid Catalytic Cracker treats the heavier, high boiling constituents from the petroleum distilling by turning them into products that are less heavy with less boiling temperatures that are more useful (Sadeghbeigi, 2000). FCC is indisputably a valuable process unit for conversion in oil processing. It is commonly employed to turn the higher molecular weight and higher boiling hydrocarbon compositions of the high value gasoline, gaseous alkenes, as well as other products (Garry & Handwerk, 2001). The fluid catalytic cracking process heats the feed to a higher temperature and relatively normal pressure, then mixed intimately with heated catalyst in powdery form. The catalysts convert to

more short gaseous molecules which are stored as vapor from high boiling long-chain hydrocarbon liquids (Dagde, 2009). Fluid catalytic cracking design affects the completion of the combustion process of the coke to the carbon dioxide in the regenerator. Flow of air for combustion is monitored in order to make available the wanted percentage of carbon monoxide (CO) to carbon dioxide for every definite fluid catalytic cracking design (Jones & Pujado, 2006). A number of reasons are responsible for catalyst to deactivate, some of which are neutralization of the acid sites by alkali metal, hydrothermal de-alumination due to high temperature and water vapour and vanadium can form a eutectic with the zeolite and cause the crystal to meet at regenerator temperature (Akah, 2017). The riser reactor of the fluid catalytic cracker unit is an integral and important part of the cracker unit where cracking operation occurs. It is where endothermic cracking operations takes place by transforming or converting heavy hydrocarbon fractions into high value lighter products. Hence, this research focused on developing transient models to predict the performance of riser reactor through the development of appropriate reaction rate expressions based on the five lump kinetic model, transient state model equations of the riser reactor to predict its dynamics and simulation of the transient model equations using kinetic parameters and industrial data to evaluate riser reactor's performance

2.0 METHOD

2.1 Rate Equation of Five Lump Scheme

The five-lump reaction scheme applied in this research is shown in Figure 1

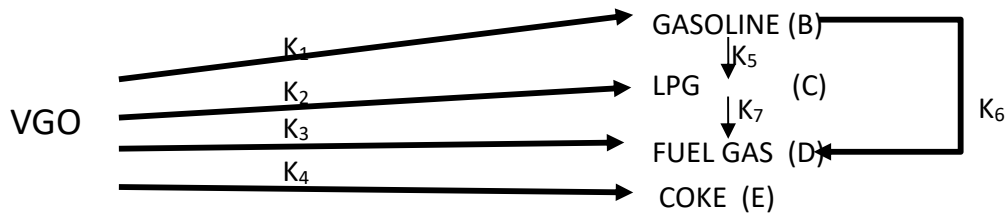


Figure 1: Five Lump Reaction Scheme

For each reaction path, the rate equation is expressed in terms of mass fraction and effectiveness factor that shows the diffusion effects of gas-oil through the zeolite catalyst pore network. The rate equations are stated thus

i. Gas Oil (A)

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

ii. Gasoline (B)

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

iii. Liquefied Petroleum Gas (C)

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

iv. Fuel Gas (D)

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

v. Coke (E)

$$-r_E = -k_4 y_A^2 \phi \eta \quad (5)$$

2.2 Riser Reactor

Fuel formation takes place in the riser reactor and this occurs within 2 to 5 seconds in the riser, thereby making available riser model equation to single dimension mass energy balances. The transient state model depicts the unsteady state behaviour of the riser reactor

2.2.1 Model Assumptions

The following assumptions are applied in developing the riser reactor model equation.

- Constant heat in the riser wall and same specific heat for coke and catalyst
- At the inlet of the riser, instantaneous vaporization takes place and catalyst gas have uniform temperature in all parts of the riser.
- Movement of fluid is not hindered by deposits of coke on the catalyst surface. Plug flow of single-dimensional transport occurs in the riser devoid of axial and radial depression.
- 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

2.2.2 Riser Reactor Material Balance Equation

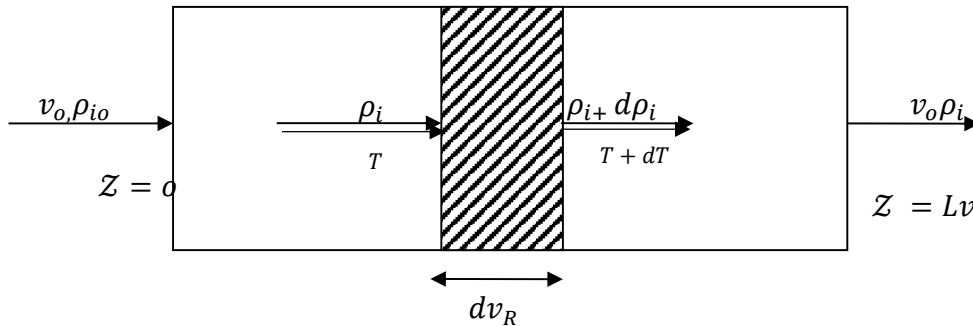


Figure 2: Riser Reactor

Through the application of conservation principle, the material balance equation is expressed thus.

Accumulation rate of mass of component i in the differential element = Inflow Rate of mass of component i into the differential element

$$- \text{Outflow rate of mass of component } i \text{ in the differential element} - \text{Disappearance Rate of mass of component } i \text{ in the differential element due to chemical reaction} \quad (6)$$

By definition of terms and upon substitution into Equation 6 yields

$$\frac{d(\rho_i v_i)}{dt} = v_o \rho_i - v_o (\rho_i + d\rho_i) - (-r_i) \rho_{gR} dv_R \quad (7)$$

Further mathematics analysis and variables substitution of Equation 7 yields

$$\frac{\partial y_i}{\partial t} + \frac{U_o \partial y_i}{\partial l} = -(-r_i) \varepsilon_R \quad (8)$$

Expressing Equation 8 in terms of dimensionless analysis

$$\frac{\partial y_i}{\partial t} + \frac{U_o \partial y_i}{L_v \partial Z} + (-r_i) \varepsilon_R = 0 \quad (9)$$

Equation 9 is the dimensionless transient model equation for plug flow riser reactor, which is defined for each reaction specie as

a. Gas Oil

$$\frac{\partial y_A}{\partial t} + \frac{U_o \partial y_A}{L_v \partial Z} + (k_1 + k_2 + k_3 + k_4) y_A^2 \phi \eta \varepsilon_R \quad (10)$$

b. Gasoline

$$\frac{\partial y_B}{\partial t} + \frac{U_o \partial y_B}{L_v \partial Z} + [(k_5 + k_6) y_B + k_1 y_A^2] \phi \eta \varepsilon_R \quad (11)$$

c. Liquefied Petroleum Gas

$$\frac{\partial y_C}{\partial t} + \frac{U_o \partial y_C}{L_v \partial Z} + (k_7 y_C - k_2 y_A^2 - k_5 y_B) \phi \eta \varepsilon_R \quad (12)$$

d. Fuel Gas

$$\frac{\partial y_D}{\partial t} + \frac{U_o \partial y_D}{L_v \partial Z} + (k_3 y_A^2 + k_6 y_B + k_7 y_C) \phi \eta \varepsilon_R \quad (13)$$

e. coke

$$\frac{\partial y_E}{\partial t} + \frac{U_o \partial y_E}{L_v \partial Z} + (k_4 y_A^2 \phi \eta \varepsilon_R) \quad (14)$$

2.2.3 Riser Reactor Transient Energy Balance

The transient energy balance model refers to unsteady state energy equation of the catalytic cracker riser reactor. The temperature distribution along the reactor can be shown by using the law of conservation of energy on a differential element of the reactor

$$\begin{aligned} &\text{Accumulation Rate of heat in the differential element} = \text{Inflow Rate of heat into the differential elements} - \text{Outflow Rate of heat from the differential element} \\ &\text{Rate of heat generated within the differential element due to chemical reaction} \end{aligned} \quad (15)$$

Upon definition of terms and substitution into Equation 15 gives

$$\begin{aligned} &\frac{d}{dt} [\rho_{gR} C_{p_{gR}} + \rho_{cat} C_{p_{cat}}] T dv = [\rho_{gR} v_o C_{p_{gR}} + \rho_{cat} v_{cat} C_{p_{cat}}] T - \\ &(\rho_{gR} v_o C_{p_{gR}} + \rho_{cat} v_{cat} C_{p_{cat}}) (T + dT) - \sum_{i=1}^n (\Delta H r_i) (-r_i) \rho_{gR} dv_R \end{aligned} \quad (16)$$

Algebraic analysis of Equation 16 and upon variable separation yields

$$\frac{\partial T}{\partial t} + \frac{(F_{gR} C_{p_{gR}} + F_{cat} C_{p_{cat}})}{(\rho_{gR} C_{p_{gR}} + \rho_{cat} C_{p_{cat}}) A} \frac{\partial T}{L_v \partial Z} = \frac{((k_1 \Delta H_{r1} + k_2 \Delta H_{r2} + k_3 \Delta H_{r3} + k_4 \Delta H_{r4}) y_A^2 \phi \eta + (k_5 \Delta H_{r5} + k_6 \Delta H_{r6}) y_B \phi \eta + k_7 \Delta H_{r7} y_C \phi \eta) \rho_{gR}}{(\rho_{gR} C_{p_{gR}} + \rho_{cat} C_{p_{cat}})} \quad (17)$$

Equation 17 is the energy balance transient model equation for riser reactor.

2.3 Solution Technique and Validation

The developed riser reactor transient model are partial differential equations in terms of dimensionless length and time. Thus, these equations are solved via the application of MatLab software and the simulated partial differential equations of the riser reactor are validated using industrial plant data of the Port Harcourt Refinery Company in predicting the riser reactor performance.

3.0 RESULTS AND DISCUSSION

3.1 Variation of Product Fractions along Reactor Length

The evaluated results from the developed transient model equations for products yield and gas oil conversion along the reactor dimensionless length is depicted in Figure 3.

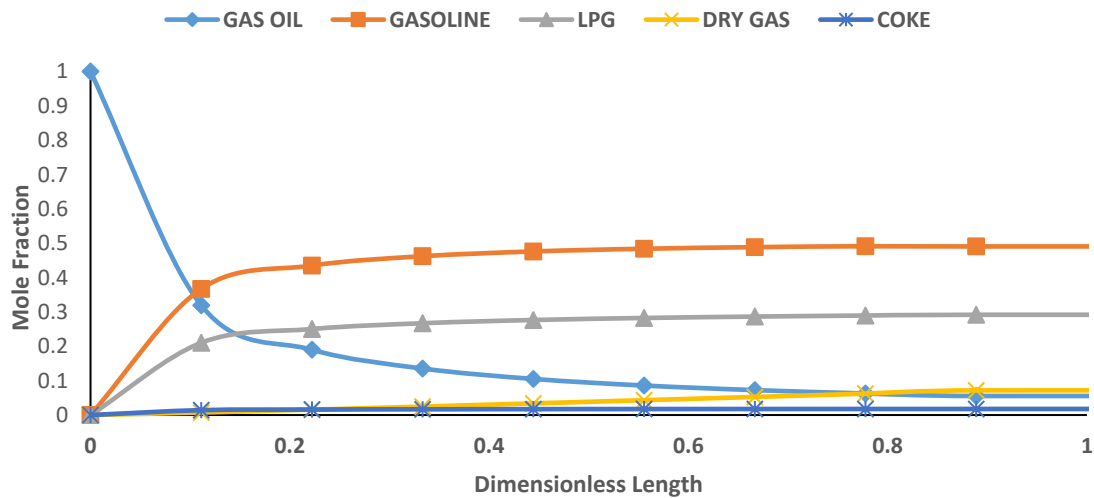


Figure 3: Feedstock and Products Yield along Reactor Dimensionless Length

The mass fraction of vacuum gas oil reduces along reactor length due to its conversion to lighter products of gasoline, LPG, fuel gas and coke. Hence, the yield of gasoline product increases to maximum while there is progressive yield of other products along the reactor dimensionless length.

3.2 Variation of Product Fractions with Time

The variation of gas oil and products yield with time are shown in Figure 4. There is gradual depletion of gas oil fraction with time as the catalytic cracking process progresses while gasoline yield increases steadily with time. Also, coke yield or production increases gradually as the reaction progresses with time.

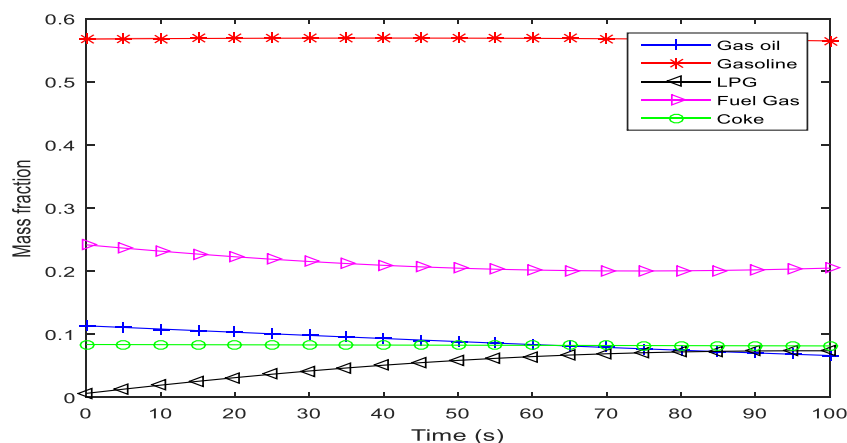


Figure 4: Feedstock and Products Yield with Time

3.3 Product Yields with Temperature

The variation of products (gasoline, liquefied petroleum gas, fuel gas and coke) mass fraction yield with temperature is highlighted in Figure 5

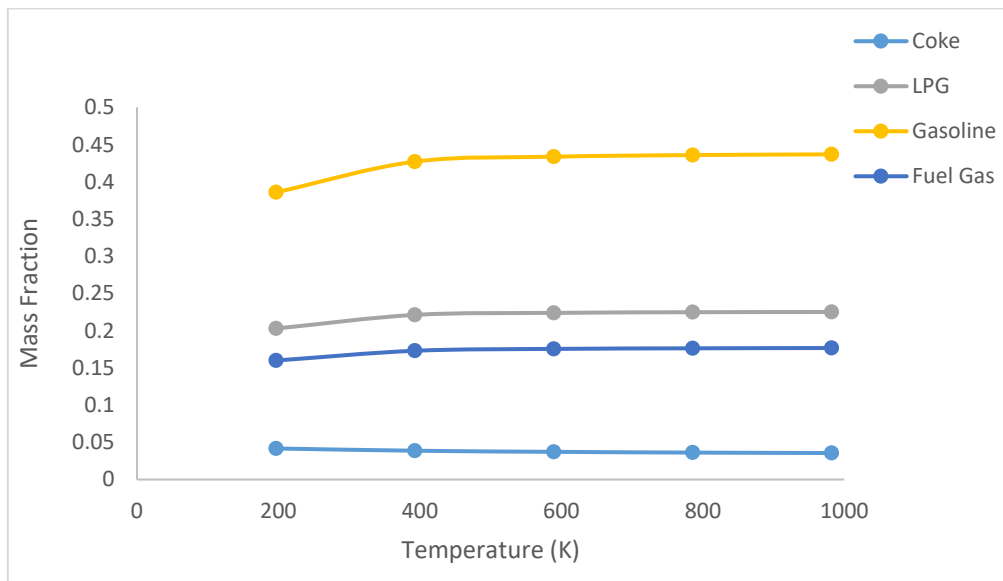


Figure 5: Products Mass Fraction with Temperature

As shown in Figure 4, higher temperature improves the endothermic cracking of gas oil to gasoline with a linear progression curve but at higher temperature, there is secondary gasoline conversion to liquefied petroleum gas and fuel gas. In addition, the yield of liquefied petroleum gas and fuel gas pointed a gradual increase and at higher temperature, there is a slight increase in their mass fraction as a result of gasoline secondary conversion. Furthermore, the temperature progression along the fluid catalytic cracking riser reactor is depicted in Figure 6 and the progressive temperature decline as a result of the endothermic cracking reaction of gas oil to valuable products.

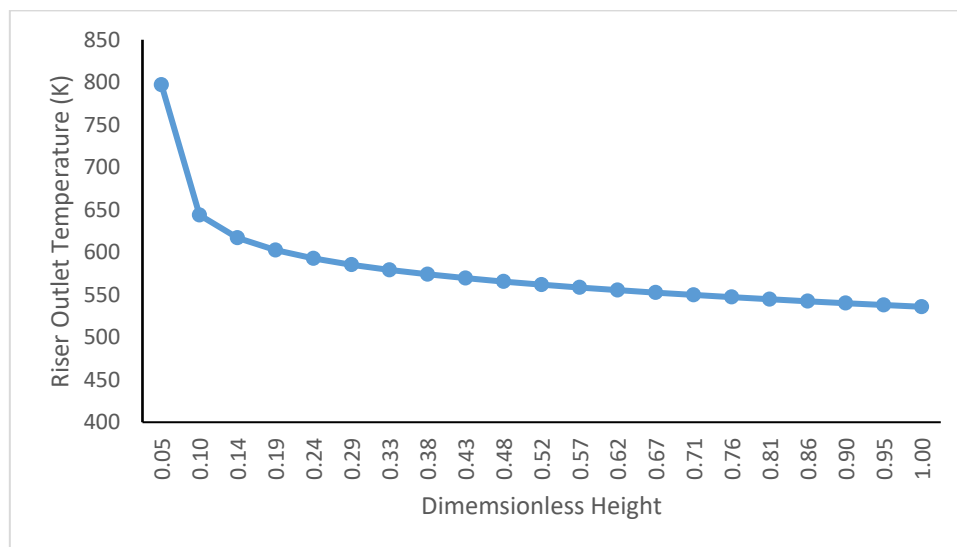


Figure 6: Temperature Progression along Reactor Dimensionless Length

4.0 CONCLUSION

This research focused on transient modeling and simulation of riser reactor of fluid catalytic cracker unit through the application of the principle of mass and energy conservativeness on a five-lump reaction scheme. The transient modeling of fluid catalytic cracker riser reactor was developed to study simulation and performance of the riser reactor, which involved cracking of vacuum gas oil to desired products via the application of material and energy balance equations. The transient model equations developed yielded a partial differential equation with respect to dimensionless length and time respectively for performance analysis of the riser reactor. Thus, the fluid catalytic cracker unit riser reactor was modelled as plug flow reactor at transient state, simulated and validated by comparing simulated transient model results with plant data.

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- [21]. **Nomenclatures**
- [22]. $k_1, k_2, k_3, k_4, k_5, k_6$ and k_7 are the intrinsic reaction rate constants
- [23]. ϕ is catalyst deactivation constant
- [24]. η is catalyst effectiveness factor
- [25]. r_A, r_B, r_C, r_D and r_E are the reaction rates of respective specie
- [26]. y_A, y_B, y_C, y_D and y_E are mass fractions of respective specie
- [27]. L_r Fluidized bed height
- [28]. ε_R Riser voidage
- [29]. l Riser length
- [30]. A_R Riser area
- [31]. t Time
- [32]. Z Dimensionless Axial distance along riser reactor