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Modeling, Kinetic Parameters Estimation and Simulation of Fluid Catalytic Cracker Reactors

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ABSTRACT
This study focuses on improvement and availability of petroleum products mainly gasoline from major refineries in Nigeria through the operation of fluid catalytic cracking unit process. Thus, steady state models were developed for fluid catalytic cracking unit that comprises of riser and regenerator reactors using five lump scheme to study their interactions. Models were developed for the fluid catalytic cracking riser reactor from the first principle as plug flow reactor and higher gasoline yield was observed for the plug flow reactor in comparison with previous study based on the effective and efficient deduction of operational kinetic parameters. Developed models were solved and simulated by estimating the five lump kinetic parameters using single point regression technique, and the estimated kinetic parameters were compared with literature data and models results compared with plant data obtained from Port Harcourt refinery Company Limited with reasonable agreement and higher gasoline yield of 56.47%, liquefied petroleum gas yield of 18.24%, flue gas yield of 15.49% and coke yield of 3.16% from the developed models due to the efficacy of estimated kinetic parameters. Also, steady state regenerator reactor was considered as two phases, bubble and emulsion phases and model developed for combustion of coke on cracking catalyst. The steady state model results for regenerator outlet temperature, coke burnt and flue gases (oxygen, carbon monoxide and carbon dioxide) are compared with industrial plant data of fluid catalytic cracking regenerator reactor with absolute minimal error
KEYWORDS: *Steady State Models, Kinetic Parameters, Simulation, Riser Reactor, Regenerator Reactor.*

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I. 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 (Obi *et al.,* 2022; Dagde, 2018). Also, per the preferred cracking reactions, development of coke transpires in these processes (Shayegh *et al.,* 2012). Throughout the process, a major percentage of the feed is transformed into coke which briefly disables the catalyst lively sites via exterminating, pore impediment, or together, occasioning in vital loss of activity. So as to reinstate the action, 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, CO_2, H_2O, SOx, and NOx compounds (Cerqueira *et al.,* 2008).

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 (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). A petroleum refining company is an engineering process plant where crude oil is treated and refined to give further valuable petroleum outputs. These include, gasoline diesel fuel, petroleum naphtha liquefied petroleum gas, kerosene, heating oil and kerosene asphalt base. In the downstream side of the industry, an oil refining plant is

recognized as a vital and integral section. These 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 remains a vital responsibility of fluid catalytic cracking (FCC), and catalytic cracker remains the password to profitability for many refiners (Ahmed *et al.,* 2014). This is so because the optimum running of the process regulates whether or not company product can keep on with today's market competition. About 350 catalytic cracking units are in operation globally, summing up a processing volume of over 12.7 million bpd. 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). The FCC unit is mostly introduced to transfigure the high-molecular weight, high-boiling hydrocarbon crude oils segments to further appreciated olefenic gases, gasoline and other products (Amino *et al.*, 2012). Originally, thermal cracking process was used to cracking petroleum hydrocarbons, but this has remained virtually entirely substituted by the fluid catalytic cracking process as it produces additional gasoline having a greater octane rating, alongside gases as by-product that have added C=C (more olefins), this makes it financially more valued than others processes via thermal cracking.

Fluid Catalytic Cracking unit is a huge unit structure with complexities at various stages of operations such as handling of solids, heterogeneous operations hydro-dynamics intricacies in the reactor (riser) and regenerator sections of the fluid catalytic cracking unit, coke depositions, coke burning kinetics and complex kinetic rates due to complex nature of feedstocks etc. Thus, FCC unit complexities with its economics importance provide reasons for extensive research study in the process of developing models and the simulation of the FCC. In addition, the importation of finished petroleum products in one of the world leading crude oil producer, Nigeria due to the inefficiencies of the conventional refineries (Ogbuigwe, 2018) is an issue of great concern. Therefore, with the government deregulation policy, thereby leading to revamping of the conventional refineries, the licensed and under construction Dangote refinery and modular refineries operations, Nigeria is focus towards self-sufficiency of finished petroleum products. Also, the FCC unit is an integral unit of conventional refining companies worldwide as this accounts for over sixty percent (60%) of these valuable products such as liquefied petroleum gas, gasoline, fuel gas, as well as coke (Dagde, 2009). Hence, the need for the development of appropriate dynamic model equations with its complexities to determine the operational mode of the FCC unit (riser and regenerator reactors).

Kinetic parameter estimation refers to the determination of the best values of critical parameters in a numerical model via assimilation of data or other similar methods. The procedure is therefore effectively applied in resolving the deficiencies of the model due to inaccuracy of parameters (Adeloye *et al.,* 2022). Hence, estimation of parameter is the method of assigning a parametric characteristic to an object, a physical operation or measurements process that are determined from that object or operation (Adeloye *et al.,* 2022; Mjalli and Ibrehem, 2011). The efficiency of material balance analysis is dependent on the accuracy of data available and the extent to which the underlying assumptions are made (Adeloye *et al.,* 2016). The estimation of kinetic parameters in a developed model plays a vital role in model's simulation and validation, thereby improving the efficiency or accuracy of the developed models in describing the characteristics of the system. The main focus of modeling an engineering operation or process is performance improvement or process of design control, thereby leading to in-depth knowledge of a process' characteristics. These parameters usually define the system stability and behavioural control, thus parameter estimation from the process data is therefore an important operation in a system model analysis (Adeloye *et al.,* 2022; Mejri *et al.,* 2018). Different techniques have been applied in estimating kinetic parameters in general, which include kinetic parameters estimation for hydrocracker reactor using five lump reaction scheme using single point regression analysis with MatLab software by Adeloye *et al*., 2022, simplex method for function minimization as a tool for kinetic parameters estimation of diesel hydrotreating process by Leandro de Rochas *et al.,* 2017 and optimization technique to obtain the best values of kinetic parameters in trickle-bed reactor process used for hydrodesulfurization of crude oil based on pilot plant experiment by Jarullah *et al.,* 2019. In addition, Sadeghi *et al.,* 2010 and Elizalde *et al.,* 2009 applied the continuous lumping model over different sets of measured data to minimize the least square error between the modeled and measured points and obtained a point estimate of the model parameters, and Kumar *et al.,* 2009 applied hybrid particle swarm optimization to estimate the continuous lumping parameter values. However, the uncertainties associated with these methods are based on unconsidered parameters data in the point estimation methods, which are the main sources of uncertainty that affects kinetic parameters estimation. These uncertainties are addressed in this study for the estimation of kinetic parameters for five lump fluid catalytic cracker unit. Therefore, the aim of this study is to develop models that predicts the steady state operation of FCC riser and regenerator reactors. This aim will be achieved by studying five lump reaction scheme of the fluid catalytic cracking feedstock, development of appropriate rate expressions, estimation of the kinetic parameters such as pre-exponential factors, activation

energy and rate constant of the reaction path, development of steady state plug flow model equations of the FCC unit thereby predicting riser products yield, outlet temperature, regenerator gaseous composition (oxygen, carbon monoxide and carbon dioxide) and catalyst regeneration (coke combustion) and performance simulation of the FCC unit (riser and regenerator reactors).

II. MATERIALS AND METHODS

The fluid catalytic cracker unit comprises of the riser reactor in which five lump reaction scheme occurs to yield various products and regenerator reactor in which the catalyst is regenerated thereby improving operational efficiency via the combustion of coke deposited on the catalyst.

2.1 Fluid Catalytic Cracking Riser Reactor

In this study, five lump reaction scheme is considered for the cracking operation in the fluid catalytic cracking riser reactor

2.1.1 Five Lumps Rate Equation

The five lumps reaction path applied in this research study is shown in Figure 1

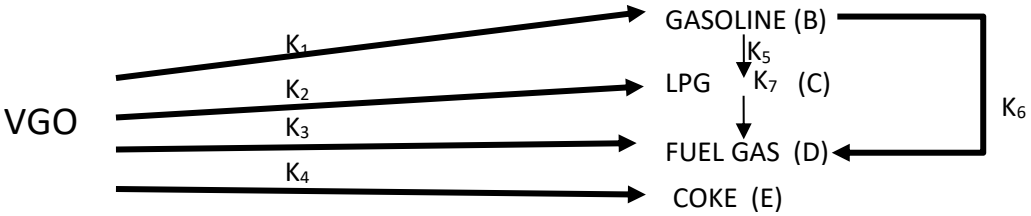

Figure 1: Five Lumps Reaction Scheme

For each component, reaction rate definition is made of mass fraction and by considering the diffusion effect of gas-oil via the Zeolite (catalyst) pore network using effectiveness factor.

a. Gas Oil (A)

$$(-r_A) = \sum_{j=1}^{4} k_j\, y_A^2 \phi\eta \quad (1)$$

b. Gasoline (B)

$$(-r_B) = \left(\sum_{j=5}^{6} k_j - \sum_{j=1} k_j\right) y_A^2 \phi\eta \quad (2)$$

c. Liquefied Petroleum Gas (C)

$$(-r_C) = \left(\sum_{j=7} k_j\, y_c - \sum_{j=2} k_j\, y_A^2 - \sum_{j=5} k_j y_B\right)\phi\eta \quad (3)$$

d. Fuel Gas (D)

$$(-r_D) = -\left(\sum_{j=3} k_j\, y_A^2 + \sum_{j=6} k_j\, y_B + \sum_{j=7} k_j\, y_c\right)\phi\eta \quad (4)$$

e. Coke (E)

$$(-r_E) = -\sum_{j=4} k_j\, y_A^2 \phi\eta \quad (5)$$

2.1.2 Steady State Riser Reactor Model

The steady state riser reactor model refers to modeling of the fluid catalytic cracking riser unit at accumulation term of zero that is time independent. In the fluid catalytic cracking unit, every reaction involving cracking takes place inside the reactor. Thus, making the riser reactor the most significant operation in the fluid catalytic cracking unit in which every reaction occurs within 2 to 5 seconds resulting from the presence of efficient feed injection system inside the FCC units. Hence, this attest to the analysis of riser reactor with a mass energy balances of single dimension (Obi *et al.,* 2022; Li and Lu, 2016; Ahari *et al*., 2008).

a. Model Assumptions

These assumptions were applied in modeling the plug flow FCC riser reactor.

i. Constant heat riser wall and same specific heat for coke and catalyst.

ii. Instantaneous vaporization occur at the riser inlet and uniform temperature of catalyst gas in all parts of the riser.

iii. Deposition of coke on the catalyst surface does not hindered fluid flow.

iv. There is no axial and radial flow of fluid but single-dimensional plug flow transport occurs in the riser.

v. There is insignificantly minimal adsorption and dispersion of catalyst particles and heat capacities and feed viscosity of all component are the same

vi. Pressure change through the riser length and the dynamics of the riser is very fast thereby ensuring a quasi-steady state model, due to the static catalyst head inside the riser

vii.

b. Material Balance Equation

By the application of the conservation principle on Figure 2 based on the assumptions highlighted above.

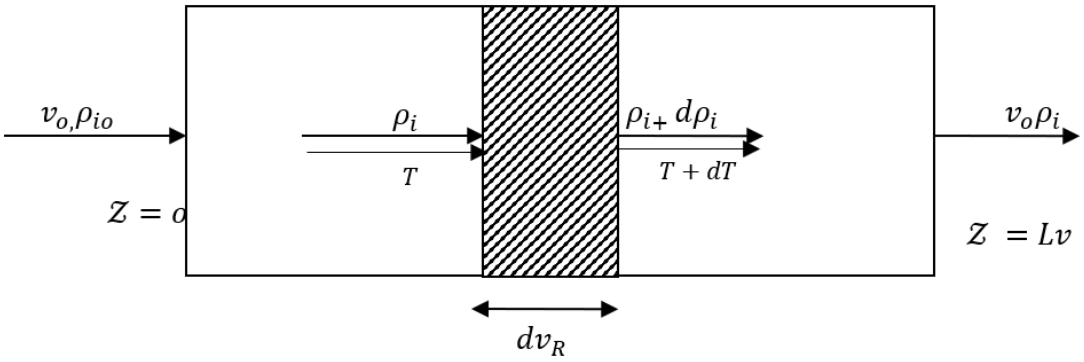

Figure 2: Plug Flow Riser Reactor

The general material balance equation in terms of dimensionless length for feedstock depletion and products yield at steady state is expressed as

$$-\frac{dy_i}{dZ} = (-r_i)\frac{\varepsilon_R L_v \rho_{gR} A_R}{F_{gR}} \quad (6)$$

Equation (6) can be written for feedstock depletion and products yield by incorporating the respective rate equation as

i. Gas Oil

$$-\frac{dy_A}{dZ} = \frac{\varepsilon_R L_v \rho_{gR} A_R}{F_{gR}} \sum_{j=1}^{4} k_j\, y_A^2\, \phi\eta \quad (7)$$

ii. Gasoline

$$-\frac{dy_B}{dZ} = \frac{\varepsilon_R L_v \rho_{gR} A_R}{F_{gR}} \left(\sum_{j=5}^{6} k_j y_B - \sum_{j=1} k_j y_A^2\right)\phi\eta \quad (8)$$

iii. Liquefied Petroleum Gas

$$-\frac{dy_C}{dZ} = \frac{\varepsilon_R L_v\, \rho_{gR} A_R}{F_{gR}} \left(\sum_{j=7} k_j\, y_C - \sum_{j=2} k_j\, y_A^2 - \sum_{j=5} k_j\, y_B\right)\phi\eta \quad (9)$$

iv. Fuel Gas

$$-\frac{dy_D}{dZ} = -\frac{\varepsilon_R L_v\, \rho_{gR} A_R}{F_{gR}} \left(\sum_{j=3} k_j y_A^2 + \sum_{j=6} k_j\, y_B + \sum_{j=7} k_j y_B\right)\phi\eta \quad (10)$$

v. Coke

$$-\frac{dy_E}{dZ} = -\frac{\varepsilon_R L_v\, \rho_{gR} A_R}{F_{gR}} \left(\sum_{j=4} k_j y_A^2\right)\phi\eta \quad (11)$$

c. Energy Balance Equation

The steady state temperature distribution along the riser reactor length can be deduced via the application of the principle of energy conservation on a differential element of the reactor shown in Figure 2. The general steady state energy equation for plug flow riser reactor in terms of dimensionless temperature and length is expressed as

$$\frac{dT_d}{dz} = -\frac{\left[\left(\sum_{j=1}^{4} k_j \Delta H_{r_j}\right) y_A^2 \phi\eta + \left(\sum_{j=5}^{6} k_j \Delta H_{r_j}\right) y_B \phi\eta + \sum_{j=7} \Delta H_{r_j} y_C \phi\eta\right] \rho_{gR} A_R \varepsilon_R L_V}{\left(F_{gR} C_{P_{gR}} + F_{Cat} C_{P_{Cat}}\right) T_{ref}} \quad (12)$$

2.2 Steady State Regenerator Reactor Model

The steady state regenerator model refers to modeling of the fluid catalytic cracking regenerator reactor at accumulation term of zero. The regenerator reactor of fluid catalytic cracking unit is grouped and model in two parts, namely.

i. **Dense Section**: The dense parts is sub-grouped into emulsion and bubble phases. The bubble phase move in plug flow and interchange heat including mass with the emulsion phase, while the emulsion phase is considered as a bed at incipient fluidization. In the dense area, combustion of the coke deposited in the dilute section is realized but complete coke combustion to carbon-dioxide is assumed in the dense region.

ii. **Dilute section:** This is the region between the top surface of the dense region and the regenerator vessel outlet. The quantity of catalyst captured in this zone is minimal compared to the overall quantity of catalyst captured in the regenerator vessel

2.2.1 Model Assumptions

The following assumptions were applied in developing the regenerator reactor model equation.

i. There is uniform temperature at every part of the dense phase in the regenerator and there is complete combustion of coke.

ii. Mass and heat interchange with the emulsion phase occurs through plug flow bubbles movement, and there is constant volumetric flow rate within the emulsion phase.

iii. Bubble phase contained only gases but no catalyst and there is no chemical reaction occurring due to very low catalyst density as a result of gas with high velocity.

iv. CO, CO_2 O_2 and N_2 only are contained in the effluent gases of the regenerator and the bed is considered to be at lowest fluidization state for catalyst in emulsion phase

v. Cyclone pipes, catalyst used and air distribution produce adequate agitation to confirm continuous stirred tank reactor character in the emulsion phase

vi. Uniform combustion of CO occurring in the bubble phase is insignificant, compared to combustion of CO in emulsion phase and there is constant flow rates of spent catalyst and regenerator catalyst

vii. Steady state operational model is applied in describing the regenerator reactor

2.2.2 Bubble Phase Gas Model

a. Bubble Phase Material Balance

The steady state bubble phase gas balance is modeled as a plug flow reactor via the principle of conservation of mass The general dimensionless steady state model equation for gases in bubble phase is expressed

$$\frac{dy_{ib}}{dL_{Gb}} = -\frac{k_{be} L_{Gss} (1-\epsilon_{bG})}{U_o} (y_{ib} - y_{ie}) \quad (13)$$

Expressing Equation (13) for respective gases yields

i. **Oxygen Gas**

$$\frac{dy_{O_2 b}}{dL_{Gb}} = -\frac{k_{be} L_{Gss} (1-\epsilon_{bG})}{U_o} (y_{O_2 b} - y_{O_2 e}) \quad (14)$$

ii. **Carbon monoxide Gas**

$$\frac{dy_{co_{2b}}}{dL_{Gb}} = -\frac{k_{be} L_{Gss} (1-\epsilon_{bg})}{U_o} (y_{cob} - y_{coe}) \quad (15)$$

iii. **Carbon dioxide Gas**

$$\frac{dy_{co_{2b}}}{dL_{Gb}} = -\frac{k_{be} L_{Gss} (1-\epsilon_{bg})}{Uo} (y_{CO_2 b} - y_{CO_2 e}) \quad (16)$$

b. Bubble Phase Energy Balance

The steady state energy balance equation for a plug flow regenerator bubble phase is expressed

$$\frac{dT_b'}{dL_{Gb}} = \frac{H_{be}L_{Gss}(1-\epsilon_{bG})}{U_b}(T_e' - T_b') \quad (17)$$

2.2.3 Emulsion Phase Gas Model

a. Emulsion Phase Material Balance

The emulsion phase reacting gases is modeled as a continuous stirred tank reactor with the principle of conservation applied at steady state. The general dimensionless steady state model equation for gases in the emulsion phase gives

$$\frac{U_{ie}dy_{ie}}{L_{Gss}dL_{GD}} = -[(-r_{iG}) + k_{be}(y_{ie} - y_{ib})](1-\varepsilon_{dG}) \quad (18)$$

Therefore, writing for respective gaseous component in the emulsion phase,

i. **Oxygen Gas**

$$\frac{U_{O_{2e}}dy_{O_{2e}}}{L_{GSS}dL_{GD}} = -\left[\left(-r_{O_{2G}}\right) + k_{be}\left(y_{O_{2e}} - y_{O_{2b}}\right)\right](1-\varepsilon_{dG}) \quad (19)$$

ii. **Carbon monoxide Gas**

$$\frac{U_{CO_e}dy_{CO_e}}{L_{GSS}dL_{GD}} = -\left[\left(-r_{CO_G}\right) + k_{be}\left(y_{CO_e} - y_{CO_b}\right)\right](1-\varepsilon_{dG}) \quad (20)$$

iii. **Carbon dioxide Gas**

$$\frac{U_{CO_{2e}}dy_{CO_{2e}}}{L_{GSS}dL_{GD}} = -\left[\left(-r_{CO_{2G}}\right) + k_{be}\left(y_{CO_{2e}} - y_{CO_{2b}}\right)\right](1-\varepsilon_{dG}) \quad (21)$$

b. Emulsion Phase Coke Balance

Applying the law of conservation of mass at steady state for coke combustion in the emulsion phase The dimensionless steady state coke balance model in the emulsion phase with no interchange of catalyst between the bubble and emulsion phase

$$\frac{dy}{L_{GSS}dL_{Gd}} = \frac{k_c y_{cG} CO_{2l} y_{O_{2e}} A_G(1-\varepsilon_{dG})}{F} \quad (22)$$

c. Emulsion Phase Energy Balance

The law of conservation of energy for gaseous components and homogenous carbon-monoxide (CO) combustion of coke on catalyst in emulsion phase at steady state. The general dimensionless steady state energy balance equation for gaseous compound in emulsion phase at constant specific heat capacity and constant volume flow rate yields

$$\frac{U_{ie}(y_{ie}-y_{ie0})C_{PG}}{L_{GSS}(1-\varepsilon_G)}\frac{dT_a}{dL_{GD}} = \sum_{i=1}^{n}(\Delta H_{ie})(-r_{ie}) + \frac{h_{be}a(T_e'-T_b')T_{ref}}{\rho_{gG}} \quad (23)$$

Thus, the dimensionless steady state energy model equation for component of gases in emulsion phase are:

i. **Oxygen Gas**

$$\frac{U_{O_{2e}}(y_{O_{2e}}-y_{O_{20}})C_{PG}dT_a}{L_{GSS}(1-\varepsilon_G)dL_{GD}} = \sum_{I=1}^{n}(\Delta H_{ie})\left(-r_{O_{2e}}\right) + \frac{h_{be}aT_{ref}(T_e'-T_b')}{\rho_{gG}} \quad (24)$$

ii. **Carbon monoxide Gas**

$$\frac{U_{CO_e}(y_{CO_e}-y_{CO_{e0}})C_{PG}dT_a}{L_{GSS}(1-\varepsilon_G)dL_{GD}} = \sum_{I=1}^{n}(\Delta H_{ie})\left(-r_{CO_e}\right) + \frac{h_{be}aT_{ref}(T_e'-T_b')}{\rho_{gG}} \quad (25)$$

iii. **Carbon dioxide Gas**

$$\frac{U_{CO_{2e}}(y_{CO_{2e}}-y_{CO_{20}})C_{PG}dT_a}{L_{GSS}(1-\varepsilon_G)dL_{GD}} = \sum_{I=1}^{n}(\Delta H_{ie})\left(-r_{CO_{2e}}\right) + \frac{h_{be}aT_{ref}(T_e'-T_b')}{\rho_{gG}} \quad (26)$$

d. Energy Balance for Solid Catalyst in the Emulsion Phase

The dimensionless steady state equation for solid catalyst in the emulsion phase of the regenerator through the application of the law of conservation of energy yields

$$\frac{U_G C_{p_{sG}}\, dT_{RG}}{(1-\varepsilon_G)l_{Gss}\, dL_{GD}} = -(\Delta H_{sG})(-r_c) \quad (27)$$

2.3 Estimation Procedures for Five Lump Kinetic Parameters

The analysis of one point regression technique applied in estimating the kinetic parameters of five lump model scheme for FCC riser and regenerator reactors are shown thus.

Step 1: Developed steady state model equations are solved numerically using MatLab software

Step 2: Simulated yield fractions of the five lump reaction paths are compared with industrial (plant) data

Step 3: Steady state yield fractions of the products are then subjected to an objective function for estimation pattern:

Estimation pattern for the objective function (S) is expressed as:

$S = (\sum_{j=1}^{m}(y_{\text{j,plant}} - y_{\text{j,cal}})^2 + (\text{T}_{R,\text{plant}} - \text{T}_{R,cal})^2)$

Subject to (Constrain functions) given as:

$y_{B0} = 0.4890;\ y_{C0} = 0.2937;\ y_{D0} = 0.0813;\ y_{E0} = 0.0177;\ T_R = 789.0471K$

$y_{i,0} > 0;\ i = A, B, C, D, E$

$y_{i,cal}$ is computed from MatLab software

The statistical test approach, that is F_{cal} as convergence or the boundary limit for the iteration estimation pattern is stated in stepwise thus;

i. $y_{i,plant}$ is obtained from Port Harcourt refinery company FCCU data. or initial boundary conditions

ii. $\bar{y}_i$ represents the mean value of y_i, that is $\bar{y}_i = \frac{\sum y_i}{n}; n = 10$

iii. Compute the total Residual Errors (SSE)

$$SSE = \sum_{i=1}^{4}((y_{iplant} - y_{ical})^2 + (T_{Rplant} - T_{Rcal})^2)$$

iv. Evaluate the Sum of Square Mean (SSM)

$$SSM = \sum_{i=1}^{4}((y_{iplant} - \bar{y}_{ical})^2 + (plant - \bar{T}_{Rcal})^2)$$

v. Compute F_{cal}

$$F_{cal} = \frac{\frac{SSM}{P}}{\frac{SSE}{n-p}} = \frac{MSM}{MSE}$$

Mean of Square Mean (MSM) = $\frac{SSM}{P}$ and Mean of Square Error (MSE) = $\frac{SSE}{n-p}$

Compute F_{tab} from 5% confidence level $(t_\propto)$

$1 - t_\propto = 1 - 0.05 = 0.95$

vi. Degree of freedom of Error (DFE) $= n - p$

vii. Compute for the corrected degree of freedom (DFM)

$DFM = P - 1$

$af = (1 - \alpha, p - 1, n - p)\ such\ that\ qf(0.95,3,23) for\ n = 10, p = 4$

F_{tab} is gotten from table of F – test on range (3,23) at 95% confidence level.

viii. Choose α such that $0 <\propto< 1$

$\propto = 0.85$

ix. Compute for new activation energies and pre-exponential factors

$E_i^{j+1} = E_i^j + \alpha\Delta s$

$k_{i0}^{j+1} = k_{i0}^j + \alpha\Delta s$

$k_i^{j+1} = k_i^j + \alpha\Delta s$

$where\ \Delta s(increment) = -(J_r J_r^T)^{-1} J_r,\ J_r\ is\ matrix\ of\ (n \times p),$

$J_r^T\ is\ transpose\ of\ J_r matrix\ (p \times n)$

Therefore $\Delta s = -[(n \times p)(p \times n)]^{-1}(n \times p)$

x. From the table of F-test, F_{tab} is determined as:

At 95% confidence level $F_{tab} = 2.278$

xi. Termination criteria

If $F_{Cal} \geq F_{tab}$, discontinue iteration and the E_i and K_{i0} values are obtained, else continues iteration till $F_{Cal} \geq F_{tab}$

xii. The estimated values of E_i and K_{i0} obtained are applied in estimating the optimal rate constants, k_i

$k_i = k_{i,0} exp\left(\frac{-E_i}{RT}\right)$

$i = A, B, C, D, E$

Step 4: The estimated rate constant values obtained are used to get optimal yield fractions of the products and feedstock depletion.

2.4 Riser Reactor Initial Condition

The feedstock being cracked to give different products is the gas-oil, the mass fraction of the product at inlet are equal to zero, gas-oil mass fraction at inlet of the reactor is unity, while at inlet, the products mass fraction equals zero. These initial conditions of the riser reactor are stated algebraically

$$Z = 0: \begin{cases} y_{Abo} = y_{Aeo} = 1 \\ y_{Bbo} = y_{Beo} = y_{Cbo} = y_{Ceo} = y_{Dbo} = y_{Deo} = y_{Ebo} = y_{Eeo} = 0 \\ T_{R(0)} = T_{ref} \end{cases}$$

III. RESULTS AND DISCUSSION

The estimated kinetic parameters (pre-exponential constants and activation energies) of the fluid catalytic cracking process using five lump scheme were compared with plant data from Dagde, 2009 in ascertaining parameters deviation or absolute error. Therefore, the comparison of plant data and estimated values of kinetic parameters (pre-exponential factors and activation energies) are highlighted in Table 1 and 2 respectively.

Table 1: Comparison of Estimated and Literature Data of Pre-Exponential Factor

Parameter	Pre-Exponential Constant (k_{i0})		Deviation
i	Plant Data	Estimated Data	(%)
1	0.00200000	0.00174000	0.13
2	0.00001824	0.0000216	0.18
3	0.00001824	0.00002024	0.11
4	0.000581	0.00055195	0.05
5	0.00005566	0.00006234	0.12
6	0.00002183	0.000017464	0.20
7	0.00317400	0.002542400	0.20

It can be deduced from Table 1 that the estimated pre-exponential factors are in reasonable agreement with the plant data with minimal deviations. Thus, its application in solving and simulating the developed model equations for fluid catalytic cracking riser reactor. Besides, the estimated activation energy values were also compared with plant data value (Dagde, 2009) to check their accuracies and applications in riser reactor simulation.

Table 2: Comparison of Estimated and Literature Data of Activation Energy

Parameter	Activation Energies (E_i)		Deviation
i	Plant Data	Estimated Data	(%)
1	46.240	36.992	0.20
2	59.750	44.813	0.25
3	59.750	41.825	0.30
4	59.750	52.580	0.12
5	78.490	57.298	0.27
6	78.490	56.513	0.28
7	59.750	50.788	0.15

Thus, there is a close convergence in the estimated and plant values of activation energies for the five lump kinetic scheme. Hence, the estimated kinetic parameters (pre-exponential factors and activation energies) are suitable in simulating the developed steady state models of the five lumps fluid catalytic cracking reactors.

4.1 Steady State Riser Reactor

In validating developed steady state model equations for feedstock depletion and products yield for five (5) lump scheme of FCC riser reactor, the result of the developed steady state model equations are analysed with plant data as shown in Table 3

Table 3: Comparison of Models and Plant Data Products Yield

Parameters	Plant Data	Model Data	Deviation (%)
Gas Oil	0.266	0.0664	0.750
Gasoline	0.459	0.5647	-0.230
Liquefied Petroleum Gas	0.17	0.1824	0.565
Fuel Gas			
Coke	0.054	0.1549	-2.794
	0.051	0.0316	-0.600

The comparison of the developed model products yield with the plant data showed higher products of gasoline, LPG, fuel gas and reduced coke production from the steady state model with more conversion of the gas oil feedstock when compared with plant data. Thus, these results can be attributed to the near accuracy of the estimated kinetic parameters data applied in simulating the models.

4.1.2 Variation of Products Fractions along Reactor Length

The result obtained from the developed models for the yield of the various output and feedstock depletion along reactor dimensionless length is shown in Figure 3.

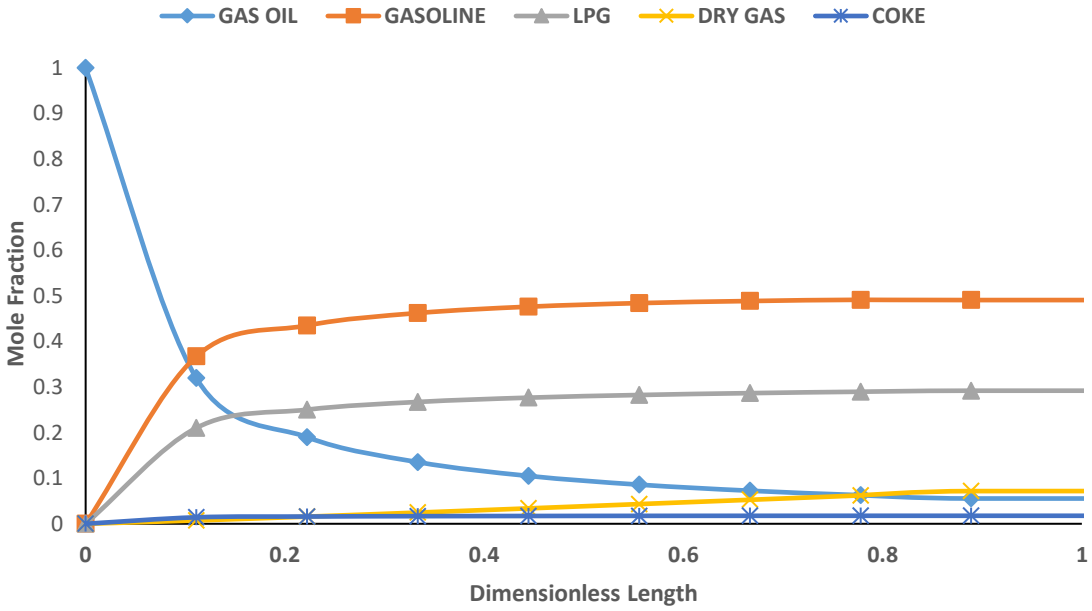

Figure 3: Variation of Feedstock and Products Yield along Reactor Dimensionless Length

It can be deduced from Figure 3 that feedstock mass fraction (vacuum gas oil) reduces along reactor length as it is been converted to lighter products of gasoline, LPG, fuel gas and coke. Thus, the yield of gasoline product increases to maximum while there is progressive yield of other products along the reactor dimensionless length. This is in conferment with the general principle of reaction rate study

4.3.1 Variation of Products Fractions with Feedstock

The effects of feedstock depletion or conversion on products (gasoline, liquefied petroleum gas, fuel gas and coke) yield was studied and analysed as depicted in Figure 4

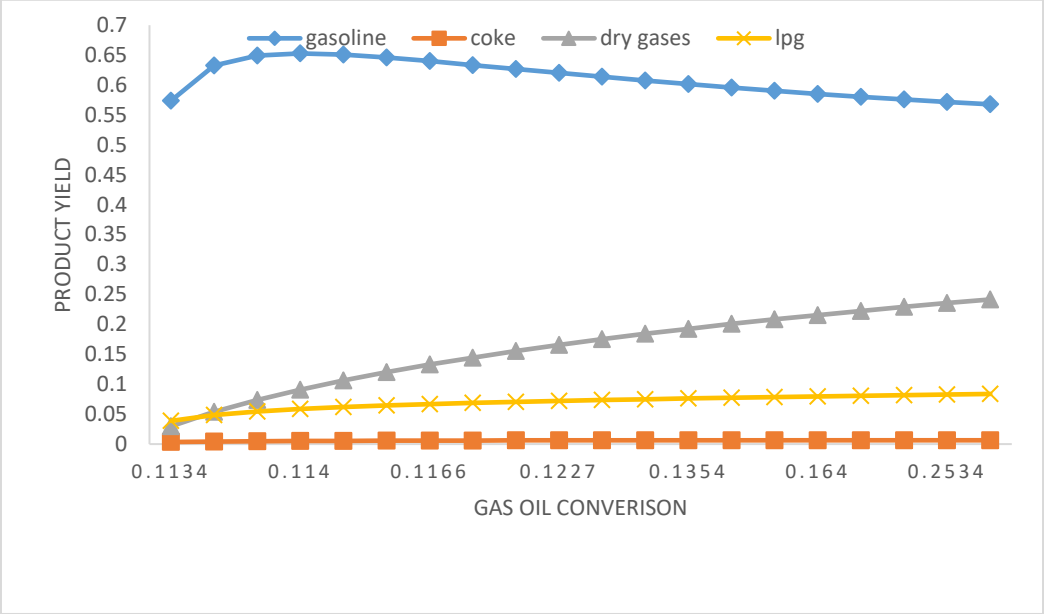

Figure 4: Variation of Products Yield with Gas Oil Conversion

It can be deduced from Figure 4 that gasoline yield increases initially with gas oil conversion and approaches to maximum and there is steady reduction as a result of gasoline cracking at high temperature range to yield liquefied petroleum gas and fuel gas respectively. In addition, the production of liquefied petroleum gas and fuel gas increases gently 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 in the fluidized bed, which ensures that a constant reactor temperature is maintained as against decline temperature progression for the riser reactor. Thus, a constant temperature throughout the bed favours the yield of liquefied petroleum gas, fuel gas and coke while the yield of desired main product (gasoline) is obtained at lower reactor height.

4.3.2 Variation of Products Fractions with Temperature

The dependency of products (gasoline, liquefied petroleum gas, fuel gas and coke) mass fraction with temperature is depicted thus.

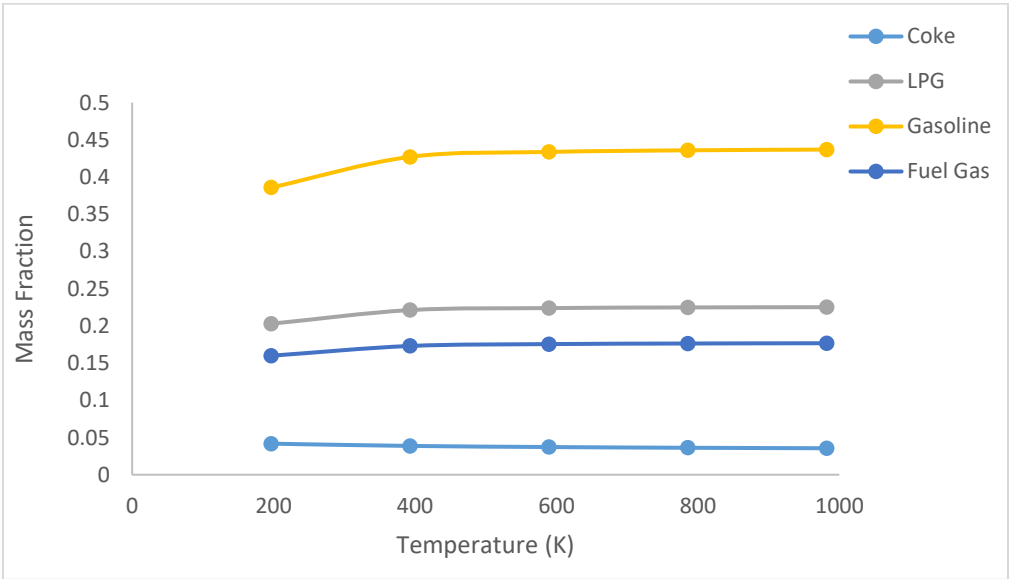

Figure 5: Variation of Products Mass Fraction with Temperature

As shown above, higher temperature enhances the endothermic cracking of gas oil to gasoline with a linear progression curve but at higher temperature, there is secondary gasoline decomposition to liquefied petroleum gas and fuel gas. Also, the yield of liquefied petroleum gas and fuel gas showed a gradual increase and at higher temperature, there is a slight increase in their mass fraction as a result of gasoline decomposition. 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.

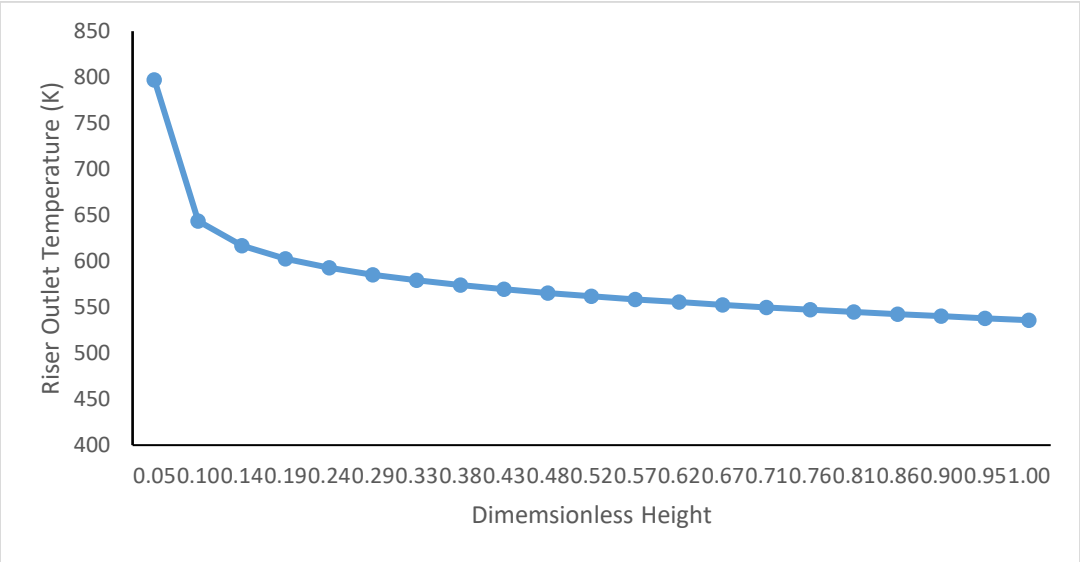

Figure 6: Temperature Progression along Reactor Dimensionless Length

4.1.3 FCC Regenerator Reactor

In validating the steady state developed models for FCC regenerator reactor, model results for regenerator outlet temperature, coke burnt and flue gases (oxygen, carbon monoxide and carbon dioxide) are compared with industrial plant data of fluid catalytic cracking regenerator reactor in Table 4.

Table 4: Comparison of Regenerator Plant and Developed Models Data

Parameters	Plant Data	Models Data	Deviation (%)
Coke (wt%)	0.007	0.00684	0.0229
Carbondioxide (mol%)	0.160	0.169	0.0563
Carbonomoxide (mol%)	0	0.051	-
Oxygen (mol%)	0.03	0.0324	0.08
Regenerator Temperature (K)	1016.48	1017.24	0.0008

The results of the developed models are generally within the plant data with 0.051 moles of CO inside flue gas as predicted by the developed model. The percentage mole of carbon monoxide predicted may not be out of range owing to the fact that the carbon monoxide generated in the plant is usually channeled to carbon monoxide boiler for generation of superheated steam and energy for the plant.

IV. CONCLUSION

This research was based on steady state modeling and simulation of fluid catalytic cracking riser and regenerator reactors using a five-lump scheme. The study focused on improvement of the limitations of previous studies of Akpa 2006; Dagde *et al.,* 2008; Dagde, 2009; Dagde & Puyate, 2012 by considering five lumps system and estimation of kinetic parameters. Hence, a steady state modeling of FCC unit was developed for efficient study and performance simulation of the riser and regenerator reactors that involved cracking of vacuum gas oil and regeneration of used catalyst in FCC unit through the application of material and energy balance equations. Also, five lump kinetic parameters were estimated using single point regression analysis and results validated by comparing with plant or literature data prior incorporation into the developed steady state model equations for the

FCC unit. The prediction and combustion of coke are of great importance in modeling and simulation of FCC unit riser and regenerator reactors, and these are achieved with five lump kinetic model. Thus, the regenerator reactor is grouped into two sections namely; dilute and dense region with focus on the dense region that comprises of bubble and emulsion phases, since the dilute region effects on the total regenerator performance is minimal and negligible.

NOMENCLATURE

$k_1, k_2, k_3, k_4, k_5, k_6$ and k_7: Intrinsic rate constants.
ϕ: Catalyst deactivation constant
η: Catalyst effectiveness factor
r_A, r_B, r_C, r_D and r_E: Reaction rate of gasoil and products formation
y_A, y_B, y_C, y_D and y_E: Mass fraction of gasoil, gasoline, liquefied petroleum gas, fuel gas an coke.
$F_{gR\ is}$ *mass flowrate of gas oil*
F_{cat} *is mass flow rate of catalyst.* v_{ob} *is the volumetric flow rate of gases into the buble phase*
ρ_{ib} *and* ρ_{ie} *are the densities of gases in the bubble and emulsion phase*
ρ_{gG} *is the rate of reaction of the various gases in the bubble phase*
K_{be} *is the interchange mass transfer cef ficient between the bubble and emulsion phases*
V_{ib} *is the volume of gases in the bubble phase*
t is the time that the gases spent in the bubble phase.
U_o: Fluid Superficial Velocity
V_{ob}: Rate of flow of gases in volume in bubble phase
ρ_{ib}: Gas density in bubble phase
$C_{p_{ib}}$: Gases specific heat capacity in bubble phase.
T_b and Te: Temperature in bubble and emulsion phases respectively
$(-r_{ib})$: Reaction rate of gases in the bubble phase
ΔH_{rib}: Heat of reaction
v_b: Volume of gas in the bubble phase
H_{be}: Bubble to emulsion phase coefficient of heat transfer
V_{ieo} *and* V_{ie}: Volumetric flow rate of gases into and out of the emulsion phase
ρ_{ieo} *and* ρ_{ie}: Densities of gases into and out of the emulsion phase
r_{iG}: Rate of reaction with respect to mass of coke and spent catalyst
L_{GD}: Dimensionless bed level

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