RESEARCH ARTICLE OPEN ACCESS

Simulation of the FCCU Regenerator Using Aspen Hysys

Digieneni Yousuo[1], Dovieme Rawlings Ighoyowho[2]

[1,2,3]Department of Chemical Engineering, Niger Delta University, P.M.B 071 Yenagoa, Bayelsa State of Nigeria.

Abstract:

Predictive simulation for process parameters during regeneration of spent catalyst in an industrial fluid catalytic cracking Unit (FCCU) are presented. The regenerator simulated model adopt a two-phase theory where the dense region of the regenerator is divided into a bubble-phase and an emulsion-phase. The emulsion-phase is simulated as a continuous stirred tank reactor (CSTR). Profiles for regenerator temperature, quantity of coke burnt and flue gas composition at different operating conditions are also presented. Simulation results indicated that the variation of inlet air flowrate have a significant influence on the performance of the regenerator. The simulation estimated optimum operating conditions of the regenerator are regenerator temperature of about 812.0oC and air flowrate of about 48023kgmole/hr which yield a complete combustion of 0.0003% of CO and a minimal coke content of 0.0064%.

Keywords— **Regenerator, coke combustion, catalyst, Aspen Hysys, Simulation.**

I. Introduction

The fluid catalytic cracking unit (FCCU) consist of the regenerator, the reactor and the fractionation column. The FCCU is where heavy oil with higher boiling point is cracked into light products. Fluid catalytic cracking (FCC) process provides 35 to 45 percent of blending stocks in the Port Harcourt refinery of gasoline pool [10].

Before, in conventional process cracking was achieved by thermal cracking process but now it has already been replaced by catalytic cracking process because of its high efficiency and selectivity i.e. gasoline is being produced with high octane number or value and less heavy fuel oils, and less light gases. The light gases produced in the process, contain more olefin hydrocarbons than those by thermal cracking process.

The cracking reactions in the catalytic reactor produces coke (carbon), which remains on the surface of the catalyst which decreases the efficiency of the catalyst and its activity decreases. To maintain the activity of the catalyst it is necessary to burn off deposited carbon on the catalyst. This was done once the regenerator and the active catalyst is further feed back to the reactor. As known, the cracking reaction is endothermic so that energy required for the process comes from the regenerator where catalyst is burned off in the presence of air which is an exothermic reaction. Some units like FCC are designed to use the supply of heat of the regenerator for the cracking purpose. The above is known as heat balance. The regenerator contains a fluidized bed catalyst (Zeolite). A controlled amount of air is supplied to the fluidized bed and the coke is burnt off the catalyst, although complete combustion is not achieved, the heat released from this reaction heats the catalyst, which in turn provides the necessary energy for cracking process in the reactor riser. Flue gas exits the regenerator through a series of internal cyclone located at the top of the system [15]. Regenerated catalyst passes from the regenerator back into the reactor. Internal cyclones are widely used in regenerator to remove catalyst particles from the flare gas stream and return these particles to the fluidized bed. Since their development in the late 1800s cyclones have become the most common mechanical separation device used in the industry [12]. Cyclones operate by rotating the entering gas stream causing the heavier particulate materials to be drawn out of the air stream, towards the outer wall of the cyclone where a laminar barrier exists. Once the particles contact this laminar region, gravitational forces cause the particles to slide down the vessel and out of the gas [6]. The controlled particles then exit through a dipleg at the bottom of the cyclone, while the exhaust gas is expelled at the top.

Cyclones are an internal part of the modern FCCU regenerator and under normal operating conditions; we have peak removal efficiency at approximately 30-40μm, allowing all particles larger than that to be fully recorded with the degree of collection of small particles depending on the type of cyclone and material in question [6]; [8]; [13]. The uses of cyclone separators to remove particles contamination still remain one of the most attractive forms available to industry. Cyclones have a lower capital investment and lower operating costs compared with cloth filtration or electrostatic precipitation [14].

Coke levels are determined by feed quality and reactor specification and alteration of the coke level will reduce increase heat generation. The change in the operating conditions will impact on the equilibrium operation of another, normally in a non-linear manner [9]. The flare gas exiting the regenerator contains catalyst materials and is released into the atmosphere. As the regenerator is the only source of catalyst emission directly into the atmosphere, this specific unit need to be studied to reduce particle emission from the FCC unit.

As discussed, heat for the cracking reaction in the riser comes from the burning off coke from the spent catalyst in the regenerator, so the temperature of the regenerator has to be regulated otherwise-selectivity of the process might take place due to overheating of the catalyst. Regulation of the regenerator flue gas containing CO_2 /CO ratio or the temperature of the regenerator can be fixed accordingly to oxygen supply controlled.

The FCC process employs a catalyst in the form of very fine particles (size of the catalyst is about 75 micrometer), which behave as fluid when aerated with vapour so here the catalyst acts as an agent for the mass transfer operation and heat transfer operation. Catalyst moves from the regenerator to the reactor and vice versa as fresh catalyst provide heat to the reactor. Usually two types of FCC units are used in industrial scale which are side by side type and ortho-flow or stacked type reactor. In side by side which will be used in this project for simulation purposes, reactor and regenerator is separated vessel placed side by side. In the case of stacked type, reactor and regenerator are mounted together.

There are so many reactions (conversion, combustion, oxidation, catalytic heterogeneous, regeneration etc.) and these reactions are sometimes not easily traceable and in order to study the complex mechanisms, reactions and process flows in the regenerator, softwares are used. Some researchers have used different softwares to simulate part of the unit [5].

In this work, the Aspen Hysys is used to study the FCC regenerator so as to predict the Optimum operating conditions of the regenerator.

II. Methodology

A. The Regenerator and its cyclones

Figure 1 shows a schematic diagram of the FCCU Regenerator while figure 2 shows the regenerator cyclones. The refinery in question utilizes a series of 12 internal cyclones, arranged in six group of two. This arrangement provides large primary cyclone to remove the majority of the particles from the air stream and allow the refinery to meet all required environmental license.

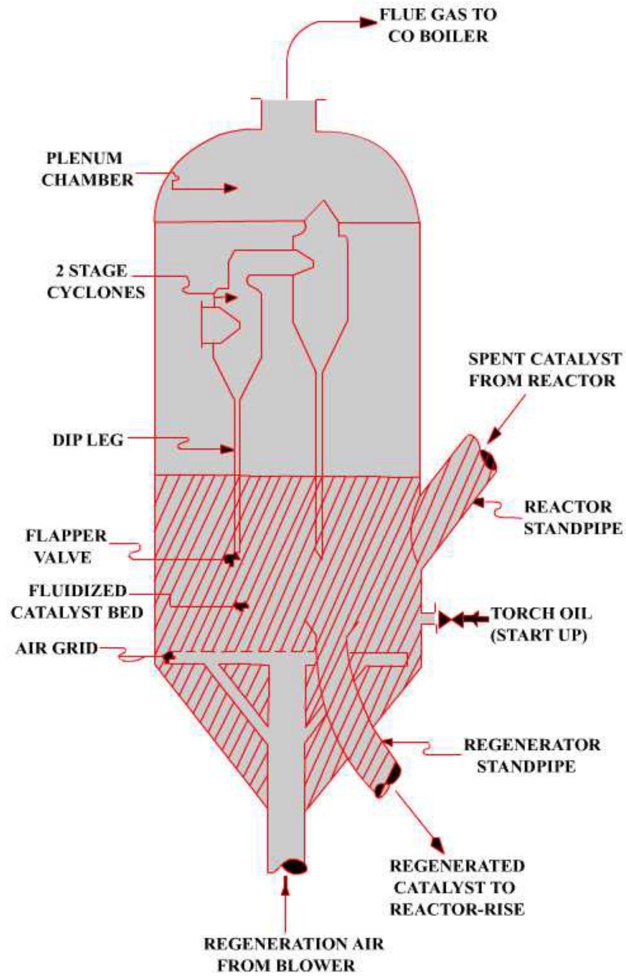

Figure 1: Schematic of FCCU Regenerator

Figure 2: Regenerator cyclone separators

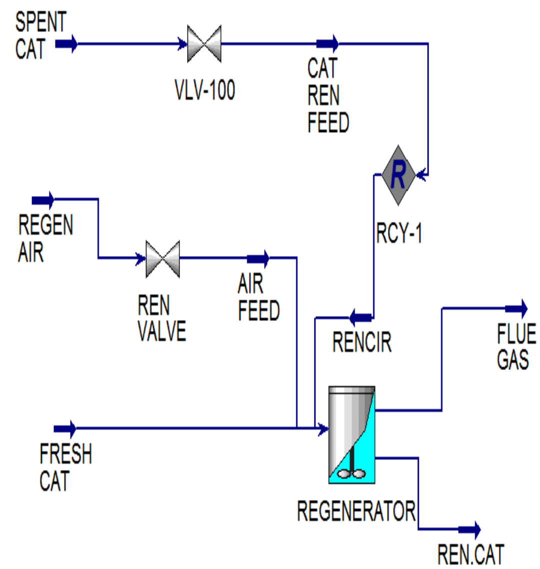

Figure 3: Model and simulated diagram of FCC Unit Regenerator.

B. The FCCU regeneration equations

Coke combustions reactions are found in the regenerator [1]. Thus during catalyst regeneration in FCC unit, coke is burnt to produce carbon monoxide and carbon dioxide [11]; [2]. Also, the homogeneous CO combustion reaction taking place in bubble-phase is assumed to be negligible compared with the catalytic CO combustion in the emissions-phase [1]; [7].Hence, the following irreversible coke reaction occurs in the emulsion phase of a regenerator [16].

Combustion reactions:

- C + $^1/_2\, O_2 \rightarrow$ CO
- CO + $^1/_2\, O_2 \rightarrow CO_2$
- C + $O_2 \rightarrow CO_2$

These are the three combustion reactions that exist in the emulsion-phase of the regenerator during combustion reactions.

C. Materials

Aspen Hysys version 8.0 was used. Operating data and piping instrumentation diagram of fluid catalytic cracking unit regenerator of the Port Harcourt refinery company (PHRC) were collected from PHRC AREA III.

D. Process Simulation

In this study, the simulation of FCC unit regenerator was developed in the simulation environment of HYSYS 8.0 software as shown in Figure 3 [3]; [4].

To present the fluid catalytic cracking regenerator in Aspen Hysys, the following steps were carried out using the aspen Hysys simulation software. The first step is mainly defining chemical components. In the Simulation Basic Manager, a fluid package was selected along with the combustion reaction set containing the three combustion reactions (RXN-1, RXN-2 and RXN-3). In the process Peng-Robinson was selected as fluid packages as it was able to handle the hypothetical components (pseudo-components). Data on carbon (coke), CO, CO_2, sulphur, nitrogen, oxygen and hydrogen are available in the Hysys component library. The Y-zeolite (Magnesiev-138) was cloned using the hypo-manager component with the data in table 1.

Table 1: Catalyst properties.

S/No	Catalyst properties	Value and Units
i.	Particle size distribution	$75 \times 10^{-6} \mu m$
ii.	Bulk density	$(0.8\ to\ 1.0)\ ^g/_{cm^3}$
iii.	Molecular weight	$162.04\ ^g/_{cm^3}$
iv.	Surface area	$200 - 300\ ^{m^2}/_g$
v.	Melting point	870^0C

The selected combustion reaction set was modelled in the regenerator with carbon and oxygen as the base components and in order to allow Aspen Hysys calculate the overall mass balance, Heat transfer of the combustion and regenerator. The data in table 2 were used in the reaction kinetics during simulation:

Table 2: Kinetics Parameter for Coke burning

Reaction	Pre-experimental constants	Activation
Coke Combustion	$1.4 \times 10^8 m^3 kmol^{-1} s^{-1}$	$224.9\,{kg}/_{mol}$
CO catalytic combustion	$247.75 m^{3(1.5)} Kmol^{0.5} s^{-1} kg^{-}$	$70.74\,{kg}/_{mol}$

The Arrhenius equation ($(K = A^{*}Exp^{(-E/_{RT})^{*}}T^{*b}$) was used, where b = 0 was assumed and the orders of the reactions were assumed to be first order. T is the reaction temperature $(200\text{-}300)^0$C and R as the ideal gas constant. The parameters in table 2 remain valid for the calculation and estimation of the reaction rate constant K_o and K_{co} used in the simulation of coke combustion reaction in the regenerator using Aspen Hysys.

In order to go to the process flow diagram (PFD) of the fluid catalytic cracking unit regenerator screen, the option "Enter Simulation Environment" was clicked. An object "Palatte" appeared at right hand side of the screen displaying various operations, streams and units.

Then materials stream (blue) was clicked to create material stream for Regenerator Air Feed, spent catalyst feed, and fresh catalyst feed imputing various compositions and conditions (temperature, flow rate and pressure) for each of the stream that was created.

The palatte was clicked and the regenerator was selected (CSTR). The dimension of the regenerator modelled was set up using the data in table 3.

Table 3: Dimension of Some component of FCC Unit [10]

Equipment	Height	Dimension
Regenerator	35.45	9.8m

The Regenerator Air Feed was fed into the regenerator at approximate flow rate of 135 KN m^3/hr, temperature 180^0C and pressure 2.5 Kg/cm^2. The fresh catalyst was fed into the regenerator at approximate flow rate 480.49 Kg/s, temperature 700^0C and pressure 0.700Kg/cm^2, and lastly the spent catalyst was fed into the regenerator at 500^0C temperature, flow rate 480.49 Kg/s and pressure 0.500 Kg/cm^2.

The main processing unit include the valves and the regenerator (CSTR). After the input information, operating unit of the regenerator were setup, the process steady-state simulation was executed by Aspen Hysys mass and energy balances of the regenerator unit.

E. Emulsion Phase Simulation

This phase is considered as a continuous stirred tank reactor (CSTR), composed of solids (catalyst and coke), air (O_2, N_2) and gases formed in the combustion (CO, CO_2, H_2O).

F. Refinery Operating Condition and Parameters of (PHRC)

The conditions stated in the tables 4 and 5 are the operating conditions obtained from the New Port Harcourt Refining Company (NPHRC) [10].

Table 4: Spent Catalyst Stream Feed Stock Composition

Components	Mass fraction (wt%)
Coke	0.05
Hydrogen	0.05
Sulphur	0
Magnesiev-138 (Y-zeolite)	0.860.9
CO	0
Nitrogen	0.02

Table 5: PHRC operating condition

Stream	Temp-erature	Pressure	Flow rate
Spent catalyst	500°C	0.500kg/cm^2	480.49kg/s
Fresh catalyst	700°C	0.700 kg/cm^2	480.49kg/s
Flue Gas	713°C	0.160 kg/cm^2	
Air	180°C	2.5 kg/cm^2	135KNm^3/hr

III. Results and Discussion

The simulation results for steady state are presented in Table 6. It shows the FCCU regenerator at various temperatures and flow rates and the corresponding simulation prediction results of CO_2, CO and Coke using the Aspen Hysis. In the simulations, the inlet spent catalyst and air flow rates are considered constant and the regenerated catalyst flow rate is made equal to the inlet fresh catalyst flow rate. The gas flow rate controls the pressure within the regenerator and it depends on the difference of pressure through the valve. A sensibility analysis regarding the inlet air flow rate and the coke fraction in the spent catalyst was conducted. These variables were chosen because of their direct influence on the rates of reactions.

Table 6: Simulation results

Air flow rate(Kg mole/hr)	Regen Temp (°C)	CO_2 (Mol.%)	CO (Mol. %)	Coke. (Wt%)
6023	627.7	0.0371	0.0236	0.4061
8523	639.7	0.0511	0.0169	0.3162
12023	656.3	0.0634	0.0115	0.2328
15023	670.3	0.0703	0.0088	0.1838
17523	681.8	0.0746	0.0072	0.1526
20023	693.1	0.0780	0.0059	0.1275
22523	704.3	0.0808	0.0049	0.1069
26523	722.0	0.0843	0.0037	0.0806
29523	735.1	0.0864	0.0030	0.0648
32023	745.9	0.0879	0.0025	0.05335
36523	765.0	0.0901	0.0018	0.0367
40023	779.6	0.0915	0.0013	0.0258
44523	798.0	0.0931	0.0007	0.0142
48023	812.0	0.0941	0.0003	0.0064
49023	816.1	0.0944	0.0002	0.0044

The graphical representation of the effect of temperature on CO_2, CO and Coke is shown in figure 4 and 5 while that of Air flow rate to CO_2, CO and Coke are shown in figure 6 and 7.

Once the catalyst is free of coke in the beginning of the simulation, there is a lack of energy generation and the temperature of the regenerator reduces (Fig.4 and 5). In this initial period, the amount of coke within the regenerator increases (Fig.5) and reaches its maximum value 0.4061% at a temperature of 627.7°C. It then reduces to 0.0064% at a temperature of 812.0°C. Coke is maximum at the point the concentration of CO is maximum (Figure 4 and 5).

In the steady state, the temperature is higher at 816.1°C and the CO mole fraction falls to a very small value that can be considered zero (Fig.4). On the other hand, the CO_2level increases with the temperature and its molar fraction stabilizes at 0.0944% (Fig.5).This happens because the constant consumption of oxygen and the temperature elevation that increases the speed of the reaction and favours the complete combustion. The variation of air flow rate was carried out to observe its influence on the combustion condition (partial or total) of the regenerator and the step change of coke fraction to verify the dependence of the regenerator transient behaviour on the step change. Some simulations were carried out with different air flow rates (Fig 6 and 7). In order to evaluate the influence of the inlet air flow on the performance of the regenerator, the simulation was carried out using different air flow rate in a steady state. The results indicate the inlet air flow rate has a direct influence on the combustion, affecting the temperature, species concentration and coke amount. Fig.6 shows the different steady state for distinct values of inlet air flow rates. As seen in Fig 7, the temperature increases to a maximum value and the CO concentration reduces to zero as the air flow rate increases. At the maximum temperature, the regenerator operation has reached its total combustion regime. Analysing the composition of the gases, one can see from partial to total combustion takes place above an air flow rate of 48023kgmole/hr.

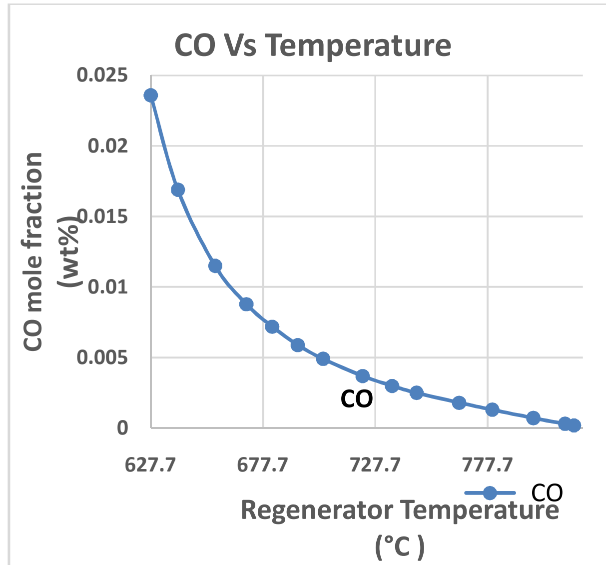

Figure 4: Effect of Temperature and CO mole fraction.

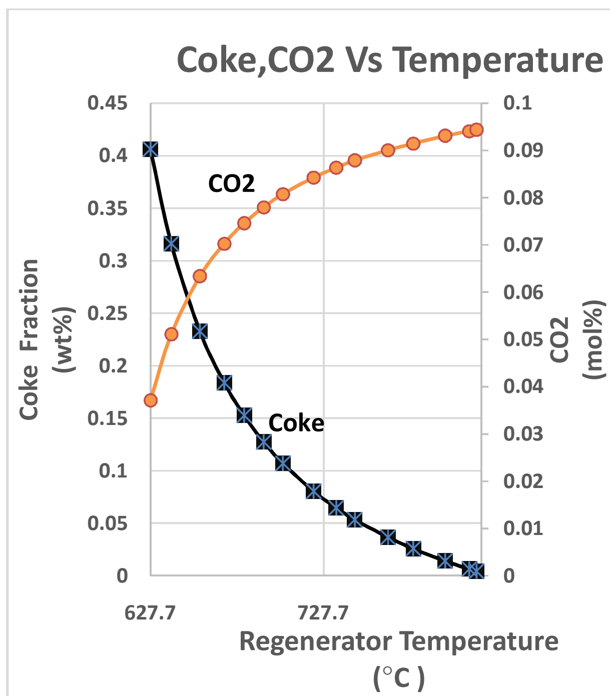

Figure 5: Effect of Temperature and CO_2 mole fraction on Coke.

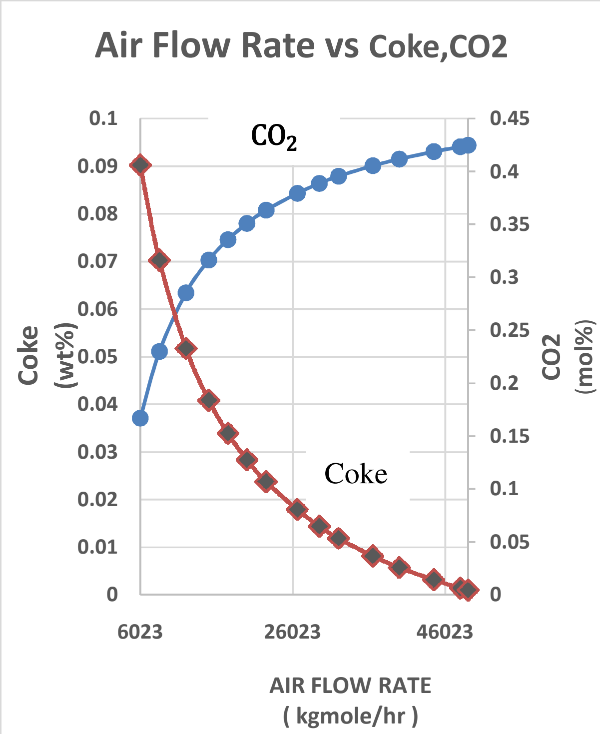

Figure 6: Effect of the air flow rate on the Coke burnt and CO_2 mole fraction.

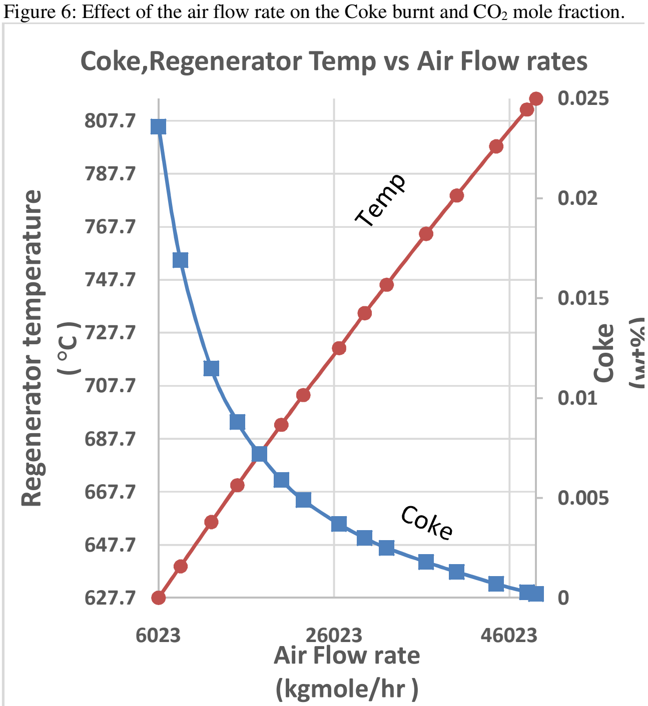

Figure 7: Effect of the air flow rate on Coke burnt and Temperature.

IV. Conclusion

The Aspen hysys simulation of the regenerator (for CSTR process) was done and the various parameters profiles were obtained. Temperature increase in the regenerator decides how much heat will flow from the regenerator to the reactor riser. The temperature increment was as a result of variation of air flow rate which produces oxygen for the combustion reaction. Combustion reaction was well established in the simulation and compositions (oxygen, carbon -dioxide, carbon and carbon monoxide) are shown accordingly. The carbon dioxide and coke mass fraction simulation results showed that there was complete combustion in the regenerator. The temperature rise was due to the combustion reaction which is governed by Arrhenius equation as stated in the methodology.

V. Nomenclature

PHRC	Port Harcourt Refining Company
CAT	Catalyst
E-cat	Equilibrium Catalyst
REN.CAT	Regenerated Catalyst
SPENT CAT	Spent Catalyst
REGEN AIR	Regenerator Air
VLV	Valve
CAT	Catalyst
RCY	Recycler
RENCIR	Recycled Spent Catalyst
CO_2	Carbon (iv) Oxide
CO	Carbon (ii) Oxide
FCCU	Fluid Catalytic Cracking Unit
NPHRC	New Port Harcourt Refining Company

References

[1] *Ali, H. and Rohani S; (1997). ''Dynamic Modelling and Simulation of Riser-Type Fluid Catalytic Cracking Unit. Chem. Eng. Tech., 20: pp118-130.*

[2] *Arbel, A. Z., Huang, Z., Rinard, I. H., Shinnar, R., Sapre, A. V. (1995). "Dynamics and Control of Fluid Catalytic Crackers-Modelling of the Current Generation FCC's", Industrial Engineering Chemical Resources, 34, pp. 1228 –1243.*

[3] *Aspen FCC User Guide. (2006), Simulation Basis, Steady State Simulation. Available in http://www.aspentech.com*

[4] *Aspen HYSYS Refining CatCracker-OpsV7 (2007), User's Manual, Aspen Tech; Inc, available in http://www.aspejntech.com*

[5] *Choi, J-H, Chang, I-Y, Shun, D-W, Yi, C-K, Son, J-E and Kim, S-D. (1999). Correlation on the Particle Entrainment Rate in Gas Fluidized Beds. Ind. Eng. Chem. Res. 38: pp2491- 2496.*

[6] *Cooper, C D and Alley, F C. (1994). Air Pollution Control Design Approach, Waveland Press, Inc: USA.*

[7] *Elnashaie, S.S.E.H., Elshishini, S.S. (1993) "Digital Simulation of Industrial Fluid Catalytic Cracking Units – IV: Dynamic Behaviour". Chemical Engineering Science, 48, pp 567-583.*

[8] *Fletcher, R, (1995). Stepwise Method Determines Source of FCC Catalyst Losses. Oil and Gas Journal 93(35).pp 8-10*

[9] *Lin, T D V, (1993). FCCU Advanced Control and Optimization. Hydrocarbon Processing 72(4): pp107-114*

[10] *NPHRC, (1987) New Port Harcourt Refinery Company: Specific Course for Senior Staff, Area 3, Process Description 1, Refinery Environmental Testing Results. Unpublished: Australia.*

[11] *Rao, T R and Bheemarasetti, J V R. (2001). Minimum Fluidization Velocities of Mixtures of Biomass and Sand. Energy 26: pp633-644.*

[12] *Ray, M B, Luning, P E, Hoffman, A C, Plomp, A and Beumer, M I L. (1997). Post Cyclone (Poc): An Innovative Way to Reduce the Emissions of Fines from Industrial Cyclones. Ind. Eng. Chem. Res. 36: pp2766-2774.*

[13] Rhodes, M. (1998). Introduction to Particle Technology, John Wiley & Sons: Australia.
[14] Schmidt, P. (1993). Unconventional Cyclone Separators. International Chemical Engineering 33(1): pp8-17.
[15] Stittig, M, (1978). Petroleum Refining Industry: Energy Saving and Environmental Control, Noyes Data Corporation: USA
[16] Weiz, P.B., Godwin, R.B. (1966) "Combustion of Carbonaceous Deposits within Porous Catalyst Particles II, Intrinsic Burning Rate". Journal of Catalysis A, 6: pp227-238.