Journal of Engineering and Applied Scientific Research
ISSN: 2384-6569
Volume 8, Number 1, 2016

THE EFFECT OF COR ON THE RISER REACTOR PERFORMANCE OF THE FCCU

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ABSTRACT: *A review on the Fluid catalytic cracking unit (FCCU) catalyst system was carried out. The riser reactor was stimulated using COMSOL Multiphysics computational fluid dynamics (CFD) software. The extra fine mesh generator of the COMSOL Multiphysics software was used to produce grid refinement in the riser reactor. The effect of catalyst oil ratio (COR) on riser reactor yields were studied. The results showed that the gasoline yield increases with the increasing COR, hold up of catalyst* $(1-\varepsilon)$ *increased with increase of COR and so for all investigated input catalyst temperature the increase of hold up can lead to higher conversion and pressure drop. A maximum on gasoline yield appears when COR is 7 making gasoline yield going up to almost 52%. A minimum on coke yield appears when COR is 5 making coke yield up to 2%.*

Keywords: CFD, COR, Cyclone, FCCU, Simulation
Received for Publication on 28 April 2016 and Accepted in Final Form 5 May 2016

INTRODUCTION

The FCCU cracking catalysts have undergone many evolutionary Changes. Milestones in cracking catalyst development are listed in table 1.0. Today's FCC catalyst system is a complex mixture of functional components. The main component is the catalyst itself, containing Y-zeolite, which provides the primary cracking function. Other components currently include the following:

i. ***Combustion promoter:*** Combustion promoters are used to reduce CO emissions and after burn in FCC regenerators.
ii. ***ZSM-5 additive:*** The ZSM-5 increases octane and light olefins yields [2].
iii. ***Desulfurization additives:*** Desulfurization additives promote oxidation of SO_2 to SO_3 in the regenerator, and adsorption of SO_3 onto alumina, which is then transferred to the riser. SO_3 is reduced in the riser and catalyst stripper to H_2S, which

is latter recovered in the gas plant

iv. ***Zeolite content:*** There has been a steady increase in zeolite content of FCC catalyst – from 10% in the 1960s to over 35% today

v. ***Zeolite type:*** There are many derivatives of Y-zeolite- basically they are $Na_{56}[SiO_2]_{136}[AlO_2]_{56}.250H_2O$. These are made by changing synthesis conditions, treatment steps, and exchange agents.

vi. ***Rare earth:*** Elements help increase the hydrothermal stability and activity of the catalyst.

vii. ***Active alumina:*** Alumina type, pore size distribution, and matrix surface area are important. Amorphous alumina was the active ingredient in cracking catalysts prior to the introduction of zeolites. While increasing bottoms conversion, amorphous alumina increases coke and gas yields.

Table 1.0: Milestones in Cracking Catalyst Development [1].

Year	Development
1942	Natural clay
1948	Microspheroidal catalyst (low alumina)
1955	Synthetic catalyst (high alumina)
1961	TCC bed catalyst (REX Zeolite)
1964	Spray-dried fluid X and Y zeolites
1974	CO combustion promoter (pt)
1975	Ni passivation additive (Sb)
1980	Coke selective Re-H-Y
1983	SO_x transfer additives
1984	Octane additive (ZSM 5)
1985	Y- zeolite improvements for low coke selectivity and higher octane.
1986-Date	Y-zeolites

METHODOLOGY

The Riser Kinetic Model

The modelling is based on the schematic flow diagram of the Port Harcourt Refinery Company (PHRC) fluid catalytic crackingg unit (FCCU) reactor presented in Figure 1 and the PHRC FCCU riser reactor in Figure 2. Figure 1 shows that The FCCU reactor consists of the riser reactor, reactor catalyst stripper, reactor separator or disengager, reactor cyclones and other auxiliary parts. Figure 1 shows among other things the boundaries of the FCCU riser reactor. The riser reactor is 33m long and the diameter is 0.8m. The ten lumps kinetic model was considered. The details of the ten lumps kinetic model are found elsewhere [7].

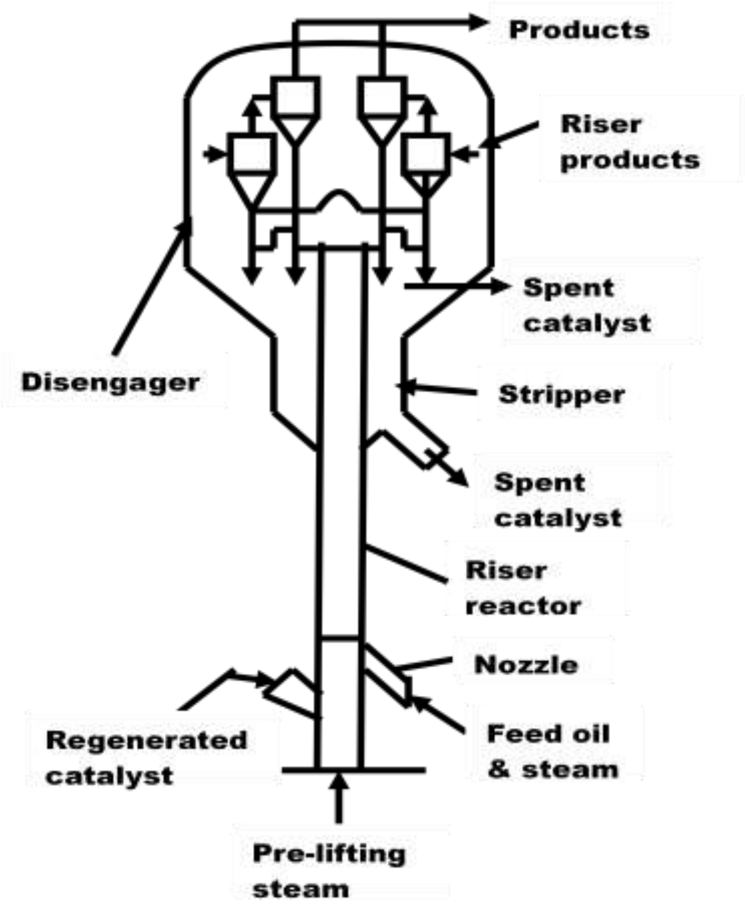
Products
Riser products
Spent catalyst
Disengager
Stripper
Spent catalyst
Riser reactor
Nozzle
Regenerated catalyst
Feed oil & steam
Pre-lifting steam

Figure 1: The PHRC FCC Reactor

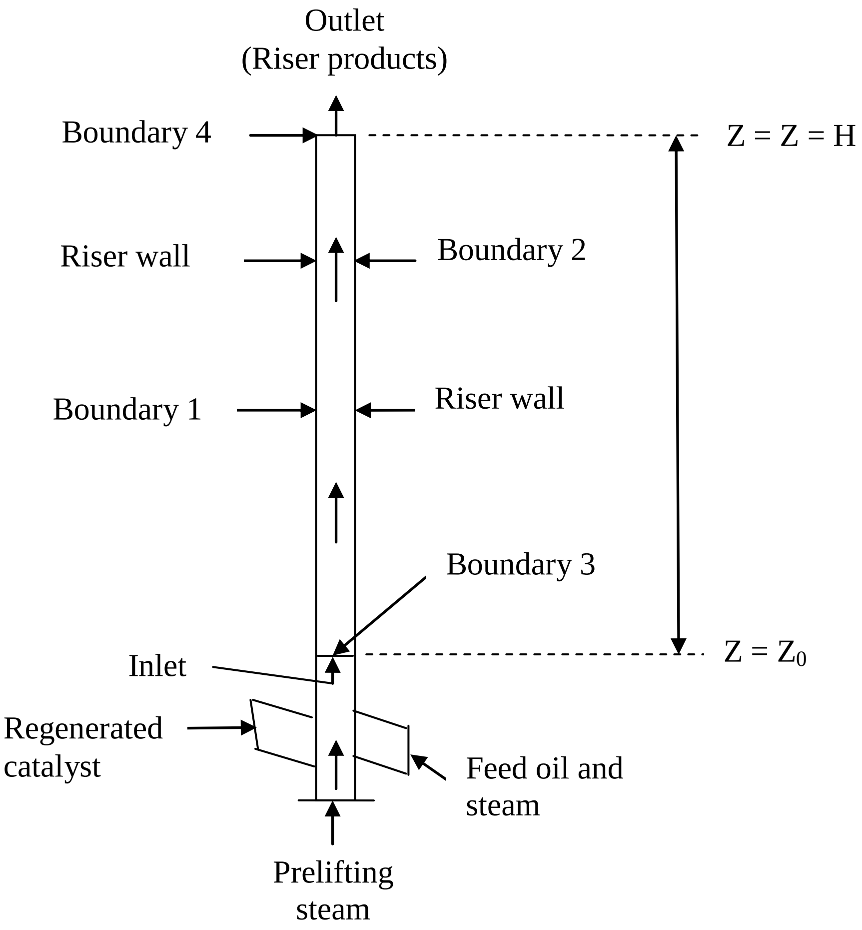

Figure 2: The PHRC FCC Riser Reactor

The Model Equations

The reactor model is an ideal plug-flow reactor, described by the mass balance in equation (1). Assuming constant reactor cross section and flow velocity, the species concentration gradient as fraction of residence time (τ) is given in equation (2). The reaction rates are given by $r_f = K_j C_i$ and to account for the different time scales, two different activity functions are used. For the non-coking reactions the activity function is given in equation (3).

$$\frac{dF_i}{dV} = \sum_j V_{ij} r_j = R_i \qquad (1)$$

$$\frac{dF_i}{dV}=\frac{d(VC_i)}{dV}=\frac{dC_i}{d\tau}=R_i \qquad (2)$$

$$a=e^{-k_d C_c} \qquad (3)$$

The reaction rates are modified by the activity according to equation (4). For the coking reactions, the activity function is given by equation (5) where α is a deactivation constant depending on the residence time. The modified reaction rates are given by equation (6). The coke content is given by equation (7) and equation (8). The values of $a, b,$ φ and α are obtained from literatures [5, 3, 6]. They are expressed as shown in equation (9) and (10) respectively.

$$r_f=aK_jC_i \qquad j=1,2,3,4,5,6,7,8,13,14,15 \qquad (4)$$

$$\boldsymbol{b = e^{-\psi t} = e^{-\alpha t}} \qquad (5)$$

$$r_f=bK_jC_i$$

$$j=9,10,11,12,16,17,18,19,20 \qquad (6)$$

$$C_c=2.43\times10^{-3}{t_c}^{0.2} \qquad (7)$$

$$Q(C_c)=\frac{1}{1+69.47(100C_c)^{3.8}} \qquad (8)$$

$$\phi=\exp(-\alpha.t_c) \qquad (9)$$

$$\alpha=\alpha_0\exp\left(\frac{-E}{RT}\right) \qquad (10)$$

For the mass transport, the inlet and outlet concentrations are obtained from equation (11) and the velocity and pressure for ideal gases are obtained from equation (12) and (13) respectively. The static head of catalyst in the riser can be calculated using equation (14). The details on chosing the void fraction variable, assumed gas velocity, slip factor and the vapourisation heat of the feed in the riser inlet are shown elsewhere [5, 6].

Inlet: $c = c_{in}$, Outlet: $c = c_{out}$ (11)

$$v=\frac{R_gT}{p}\Sigma F_i \qquad (12)$$

$$p=R_gT\sum C_i \qquad (13)$$

$$-\frac{dp}{dz}=\rho_{cat}g.(1-\varepsilon) \qquad (14)$$

For momentum transport, the inlet and outlet pressure are obtained from equation (15)

$$p=p_{in}-\rho_{cat}g(1-\varepsilon)(z-z_0) \qquad (15)$$

For energy balance, neglecting pressure drop, the energy balance for an ideal reacting gas, as well as an incompressible reacting liquid is given by equation (16) and (17). The inlet temperature is calculated putting into consideration the energy balance of the components. Equation (18) is used in calculating the inlet temperature while equation (19) is used for calculating the outlet temperature.

$$\sum_i M_iC_{p,i}\frac{dT}{dV}=w_s+Q+Q_{ext} \qquad (16)$$

$$Q=-\sum_j H_jr_j \qquad (17)$$

At $z = z_0 = 0$, $w_s = 0$, $Q_{ext} = 0$, equation (16) and (17) becomes

$$\sum_i M_iC_{p,i}\frac{dT}{dV}-Q=0$$

This implies that

$$M_{cat}.Cp_{cat}.(T-T_{cat})+M_{go}.Cp^{l}_{go}.(T_{vap}-T_{go})+ M_{go}.Cp^{v}_{go}.(T-T_{vap})+M_{go}.\Delta H_{vap} +M_{ds}.CP_{ds}.(T-T_{ds})=0$$

That is

$$T_0=\frac{(M_{cat}Cp_{cat}T_{cat})-(M_{GO}Cpl_{GO}(T_{vap}-T_{GO}))+(M_{GO}Cpv_{GO}T_{vap})-(M_{GO}\Delta H_{vap})-(M_{ds}Cp_{ds}T_{ds})}{M_{cat}Cp_{cat}+M_{GO}Cpv_{GO}+M_{ds}Cp_{ds}} \quad (18)$$

At z = h or z, w_s = 0, Q_{ext} = 0, equation (16) and (17) becomes

$$\sum_i M_i C_{p,i}\frac{dT}{dV}=Q$$

That is, $\sum_i M_i C_{p,i}\frac{dT}{dV}=-\sum_j H_j r_j$

This implies that $\boldsymbol{T_z-T_0=-\frac{\sum_j H_j r_j}{\sum_i M_i C_{p_i}}dv=-\frac{\sum_j H_j r_j}{\sum_i M_i C_{p_i}}(\pi D)(z-z_0)}$

That is, $\boldsymbol{T_z=T_0-\frac{\pi D\sum_j H_j r_j}{\sum_i M_i C_{p_i}}z}$

By our correlation $\boldsymbol{T_z=T_0-\frac{\pi D\sum_j H_j r_j}{\sum_i M_i C_{p_i}}z}$ is

$\boldsymbol{T_z=T_0-0.55*z}$ or $\boldsymbol{T_0-7.7*t\text{^}0.35}$ hence

Outlet: $T=T_z=T_0-7.7*t\text{^}0.35$ (19)

Boundary Conditions

The boundary conditions for the riser reactor are shown in table 2.

Table 2: Boundary Conditions

SETTINGS	BOUNDARY	BOUNDARY	BOUNDARIES
	3	**4**	**1 and 2**
Temperature			
Boundary type	Inlet	outlet	wall
Boundary condition	Temperature	Temperature	Thermal insulation
Value	T_0	T_n	-
Concentration			
Boundary type	Inlet	outlet	wall
Boundary condition	Concentration	Concentration	Insulation/Symmetry
Value	c_{in} for all species	c_{out} for all species	-
Velocity and pressure			
Boundary type	Inlet	outlet	wall
Boundary condition	Velocity	Pressurre, no viscous stress	No slip
Value	$w_0 = v_s$, $u_o = v_0 = 0$	P_0 = P-n	-

MATERIALS

The average molecular weights, the thermodynamic properties of the feed, the plant operating conditions and the properties of the catalyst used in this study, the specific heat of different lumps and the kinetic parameters for cracking reactions are shown in table 3 to 7 and others are found elsewhere [4, 5, 3].

Table 3: Riser Dimensions

	Length (m)	Diameter ((m)
Riser reactor	33	0.8

Table 4: Average Molecular Weight and Heat Capacities [3]

Species	MW (kg/kmol)	Cp (kJ/kg.K)
Gas oil	333.0	2.67(liquid), 3.3(Gas)
Gasoline	106.7	3.3
Light gases	40.0	3.3
Coke	14.4	1.087
Steam	18.0	1.9
Catalyst	N/A	1.087

Table 5: Thermodynamic Properties of the Feed

Gas oil vaporization temperature	698K
Viscosity of gas	1.4 x 10-3 N.S/m2
Gas oil enthalpy of vapourisation	190 kJ/kg

Table 6: PHRC Plant Operating Conditions [4]

Feed rate (kg/s)	30.87
Feed Quality (API)	D1298
COR (kg/kg)	7.04
Inlet pressure (kPa)	221
Feed temperature (K)	505
Catalyst inlet temperature (K)	1004
Steam (wt%)	5
Steam temperature (K)	464
Catalyst density (kg m−3)	840
Gas density (kg m−3)	5.3
Gas velocity (m sec−1)	2.5

Table 7: Kinetic Data for the Cracking Reactions [5]

Cracking Reaction	Activation energy (kJ/mol)	Freequency factor (hr^{-1})	Rate at 538^{0}C (hr^{-1})	Molecular weight of cracking lump
HFO to LFO	60.7086	1.422 x 10^7	1760.4	380
HFO to gasoline	23.0274	1.026 x 10^5	3380.4	380
HFO to coke	73.269	3.704 x10^7	712.8	380
LFO to gasoline	23.0274	8.215 x 10^4	2707.2	255
LFO to coke	73.269	1.852 x 10^7	356.4	255
Gasoline to coke	41.868	8.555 X10^4	172.8	120
Gas oil to gasoline	68.2495	7.978 x 10^5	39.364	380
Gas oil to gas	89.2164	4.549 x 10^6	9.749	380
Gas oil to coke	64.5750	3.765 x 10^4	6.012	380
Gasoline to gas	52.7184	3.255 x 10^3	2.470	120
Gasoline to coke	115.4580	7.957 x 10^1	1.364	120

Mesh Generation and Simulation

The extra fine mesh generator of the COMSOL Multiphysics software was used to produce grid refinement in the riser reactor. The riser reactor was meshed into 77,358 triangular elements. Figure 3 shows the computational grid used to represent the computational domain of the riser reactor. The simulations in this work used the 3-dimensional model of the COMSOL multiphysics CFD software in a windows vistaTM Home Premium; model: HP Pavilion dv 6500 Notebook PC, Processor: Intel (R) Core(TM)2 Duo CPU T5450 @ 1.66GHz - 1.67GHz, Memory (Ram): 250GB and System type: 32-bit operatin system.

RESULTS AND DISCUSSION

The Effect of the COR on the Riser Reactor Performance

The catalyst oil ratio (COR) is very important parameter in FCC process. The gasoline yield increases with the increasing COR (Figure 3.0). Hold up of catalyst (1-ε) increased with increase of COR, so for all investigated input catalyst temperature (Figure 4.0), the increase of hold up can lead to higher conversion and pressure drop (Figure 5.0).

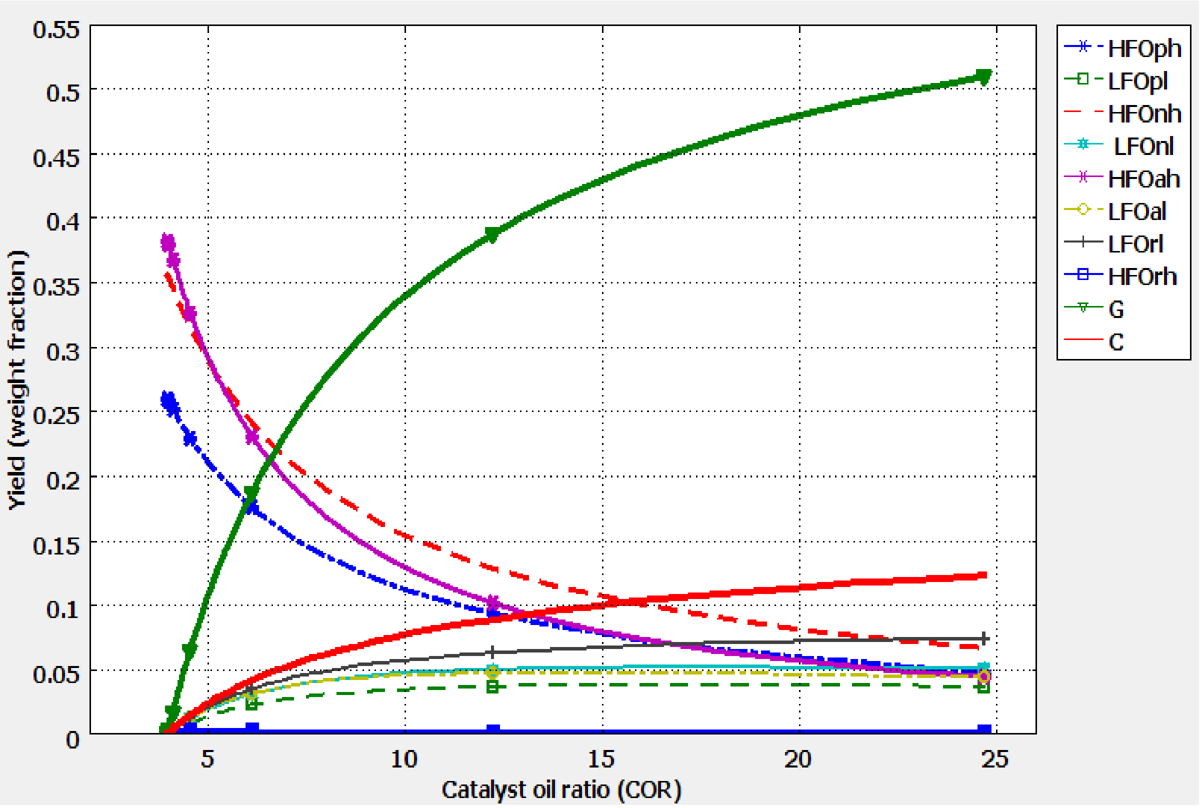

Figure 3.0: The Effect of Catalyst Oil Ratio (COR) on Yield.

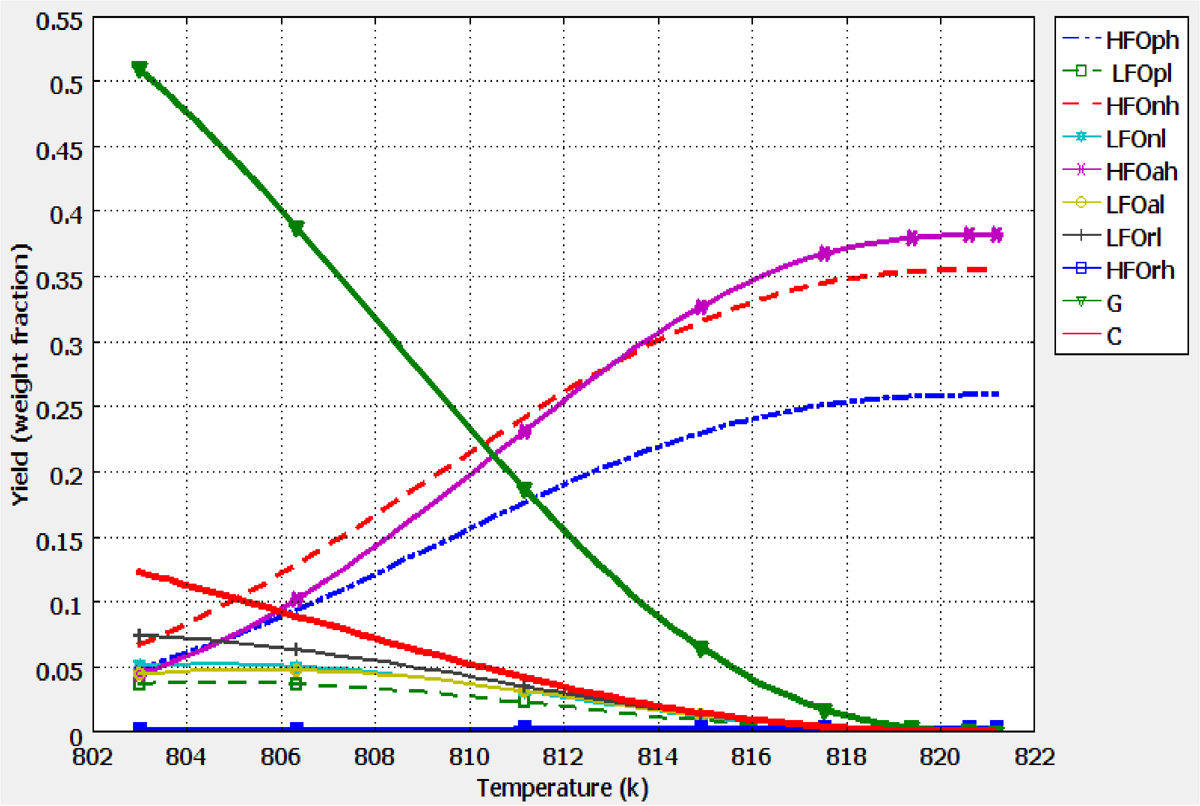

Figure 4.0: The Effect of Changing Inlet Temperature on Yield

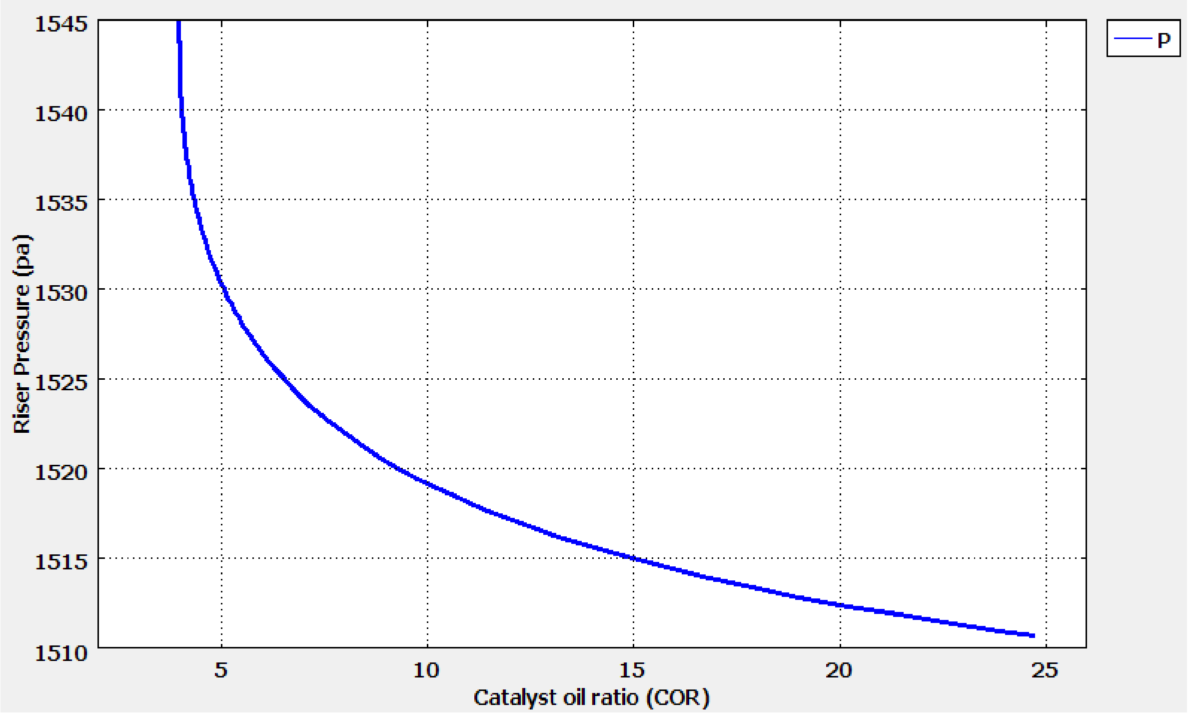

Figure 5.0: The Riser Pressure Versus Catalyst Oil Ratio (COR)

Figures 6.0 and 7.0 are 3-D graphics of the impact of variations of COR on FCC yields. The ten lump model is used in order to illustrate our results for a heavy gasoil. The effect of catalyst oil ratio (COR) on gasoline yield is given in figure 6.0. A maximum on gasoline yield appears when COR is 7 making gasoline yield going up to almost 52%.

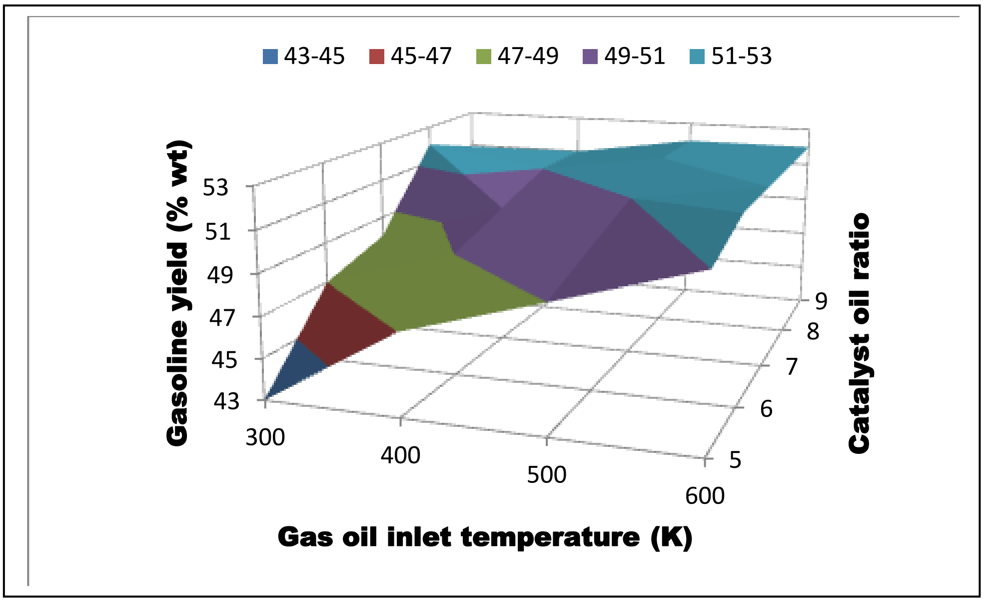

Figure 6.0: Effect of Catalyst Oil Ratio (COR) on Gasoline Yields

Figure 7.0 shows the effect of catalyst oil ratio on coke yield. At COR of 7, Coke (C_1- C_4 + coke) yield is 15% by weight. That is C_1- C_4 yield is 7.5% by weight and coke yield is 7.5% by weight. A minimum on Coke yield appears when COR is 5 making coke yield up to 2%.

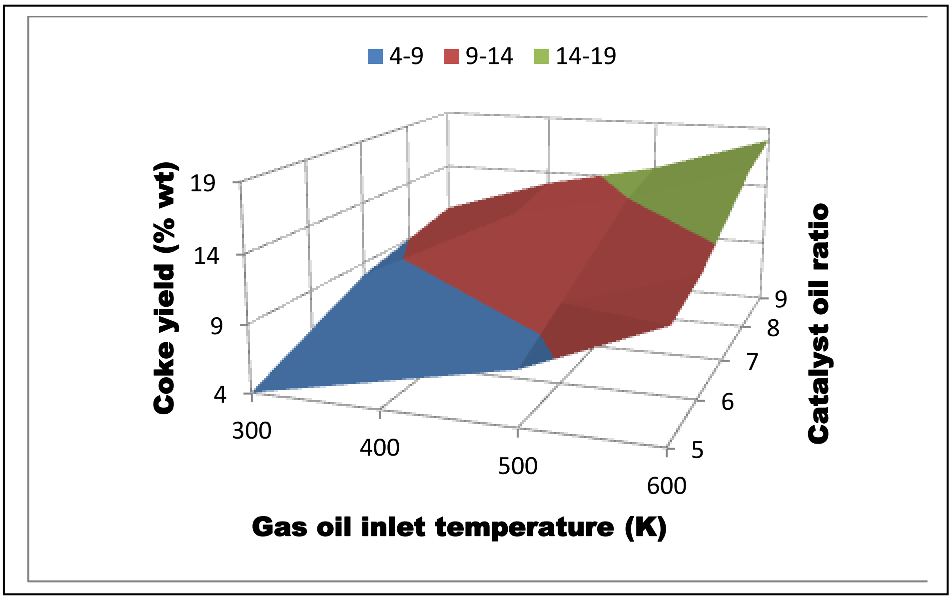

Figure 7.0: Effect of Catalyst Oil Ratio (COR) on Coke Yields

CONCLUSION

The FCCU riser reactor has been simulated using COMSOL Multiphysics CFD software. The effect of catalyst oil ratio (COR) on riser reactor yields were studied. The results showed that COR affects the yield of gasoline, coke and other cracked products. The results also revealed that the gasoline yield increases with the increasing COR, hold up of catalyst (1-ε) increased with increase of COR and so for all investigated input catalyst temperature the increase of hold up can lead to higher conversion and pressure drop. A maximum on gasoline yield appears when COR is 7 making gasoline yield going up to almost 52%. A minimum on Coke yield appears when COR is 5 making coke yield up to 2%.

Nomenclature

The nomenclature is given in table 8.

Table 8: Nomenclature

c:	Concentration, mol/m^3		Mass flow rate of catalyst, kg/s
E:	Activation energy for rate constant, J/mol	P_{in}:	Inlet pressure, pa
g:	Acceleration due to gravity, m/s^2	Rg (R_u):	Gas constant, J/(mol.K)
P:	The pressure of gases, pa	T_{cat}:	Temperature of the catalyst, K
R, r:	Rate expression value	ε:	Void fraction
T:	Tempersature, K	T_{go}:	Temperature of gas oil, K
t, τ:	Residence time, s	T_{vap}:	Gas oil vapourization temperature, K
v:	Volume, m^3	v_0:	Outlet velocity, m/s
z:	Axial distance from the inlet, m	T_{ds}:	Temperature of the steam, K
CP_cat	(Cp_{cat}): Specific heat of catalyst, J/kgK	V_R, υ, V:	Reactor volume, m^3
Cp_ds(Cp_{ds}):	Specific heat of steam, J/kgK		
CpL_GO ($CP^L go$):	Specific heat of liquid gas oil,		

J/kgK

CpV_GO ($CP^V go$): Specific heat of gaseous gas oil, J/kgK

$C_{i:}$ Species molar concentrations, mol/m^3

$c_{in:}$ Inlet concentration, mol/m^3

$c_{out:}$ Outlet concentration, mol/m^3

K_d: Deactivation constant

M_go (M_{go}): Mass flow rate of gas oil, kg/s

M_ds (M_{ds}): Mass flow rate of steam, kg/s

$W_{s:}$ Additional work term

Q: Heat due to chemical reaction, J/m^3.s

$Q_{ext:}$ Heat added to the system, J/m^3.s

μ: Viscosity, N.S/m^2

ρ: Density, Kg/m^3

Ψ: Slip fact

Subscripts

j: Refers to lump j that is cracked

i: Refers to lump i that is formed

p (or s): Particle/solid

a (or f): Air/fluid

cat: Catalyst

c: Coke content

Table 8: Nomenclature

c: Concentration, mol/m^3

E: Activation energy for rate constant, J/mol

g: Acceleration due to gravity, m/s^2

P: The pressure of gases, pa

R, r: Rate expression value

T: Tempersature, K

t, τ: Residence time, s

v: Volume, m^3

z: Axial distance from the inlet, m

CP_cat (Cp_{cat}):Specific heat of catalyst, J/kgK

Cp_ds(Cp_{ds}):Specific heat of steam, J/kgK

CpL_GO ($CP^{L}go$): Specific heat of liquid gas oil, J/kgK

CpV_GO ($CP^{V}go$): Specific heat of gaseous gas oil, J/kgK

$C_{i:}$ Species molar concentrations, mol/m^3

$c_{in:}$ Inlet concentration, mol/m^3

$c_{out:}$ Outlet concentration, mol/m^3

K_d: Deactivation constant

M_go (M_{go}): Mass flow rate of gas oil, kg/s

M_ds (M_{ds}): Mass flow rate of steam, kg/s

M_cat (M_{cat}): Mass flow rate of catalyst, kg/s

$P_{in:}$ Inlet pressure, pa

Rg (R_u): Gas constant, J/(mol.K)

T_{cat}: Temperature of the catalyst, K

ε: Void fraction

T_{go}: Temperature of gas oil, K

T_{vap}: Gas oil vapourization temperature, K

$v_{0:}$ Outlet velocity, m/s

T_{ds}: Temperature of the steam, K

V_R, υ, V : Reactor volume, m^3

$W_{s:}$ Additional work term

Q: Heat due to chemical reaction, J/m^3.s

$Q_{ext:}$ Heat added to the system, J/m^3.s

μ: Viscosity, N.S/m^2

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Reference to this paper should be made as follows: Yousuo Digieneni (2016), The Effect of COR on the Riser Reactor Performance of the FCCU. *J. of Engineering and Applied Scientific Research,* Vol. 8, No. 1, Pp. 30 – 41.