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Application of COMSOL Multiphysics in the Simulation of the Fluid Catalytic Cracking Riser Reactor

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Abstract:

The Fluid Catalytic Cracking (FCC) riser reactor of the Fluid Catalytic Cracking Unit (FCCU) was studied and simulation was carried out using COMSOL Multiphysics Computational Fluid Dynamics (CFD)) software. The 20-lump kinetic model was used to describe the kinetics of the cracking reactions in the riser reactor. The predicted results of the yields of products from the riser reactor were compared using practical values from Refinery plants as in [2], [8]. The results show that in all cases of comparison, the deviation is minimal (±10% for gasoline and coke yields while the output temperature is ± 20k). This implies that COMSOL Multiphysics software can be used to predict the yields and output temperature of the riser reactor accurately.

Keywords- **COMSOL, FCCU, Kinetics, Multiphysics, Reactor, Riser, Simulation, Yields.**

I. Introduction

Modern refinery has many units. Fluid catalytic cracking unit (FCCU) is one of them and it is the workhorse of modern refinery. The Fluid catalytic cracking unit (FCCU) converts heavy petroleum fractions using catalyst into more usable products such as gasoline, middle distillate and light olefins as in [10], [4], [12], [5], [6]. The FCC reactor is one of the most complex equipment in the refinery. The FCCU reactor consists of the riser reactor, reactor catalyst stripper, reactor separator or disengager, reactor cyclones and other auxiliary parts. Most of the reactions in the FCC reactor occur in the FCC riser reactor.

The riser reactor is one of the most important units in the FCC process, which is widely used in the modern petroleum refinery industry. A riser reactor can be divided into four parts from bottom to top according to their functions: the prelifit zone, the feedstock injection zone, the full-reaction zone, and the quenching zone. A detail work on riser parts description, diameter, height, residence time and configuration as shown in [12], [4], [14].

COMSOL Multiphysics is a powerful interactive environment for modeling and solving all kinds of scientific and engineering problems based on partial differential equations (PDEs). With this software you can easily extend conventional models for one type of physics into multiphysics models that solve coupled physics phenomena—and do so simultaneously. A more detailed description of this mathematical and numerical foundation appears in [1], [13].

In this study, COMSOL Multiphysics software was used to simulate the FCC riser reactor of the FCCU. The 20-lump kinetic model was used to describe the kinetics of the cracking reactions in the riser reactor in order to compare the yield with existing data from plants as in [2], [8]. Detail work on kinetic lumping is reported in [11], [7], [4], [9], [2], [5], [6], [3], [14].

II. Methodology

A. The riser reactor equations

Figure 1 shows the FCC reactor which consists of the riser reactor, reactor catalyst stripper, reactor separator or disengager, reactor cyclones and other auxiliary parts. Figure 2 is the riser reactor and its auxiliary parts. The model equations used was based on the schematic flow diagrams of the riser reactor as presented in Figure 3. The riser reactor is

33m long and the diameter is 0.8m. The 20 lumps of pseudo components are presented in table 1.0 and the corresponding 190 rate constants from the 20 lumps as they undergo cracking are shown in table 2.0 and details are shown in [13].

In table 1 and 2, some of the components in one lump may appear the same as that of another in their uses but can be only differentiated with some parameters like their boiling points, their molecular weight, their heat of combustion, etc are in [5], [13], [14]. In table 2 row 1, L1 can be cracked to L2, L3, L4, L5, L6, L7, L8, L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19 and L20 and the corresponding rate constants are K_{12}, K_{13}, K_{14}, K_{15},

K_{16}, K_{17}, K_{18}, K_{19}, K_{110}, K_{111}, K_{112}, K_{113}, K_{114}, K_{115}, K_{116}, K_{117}, K_{118}, K_{11} and K_{120}. The other cracked products and there corresponding rate constants are as shown from row 2 to row 20 in table 2.

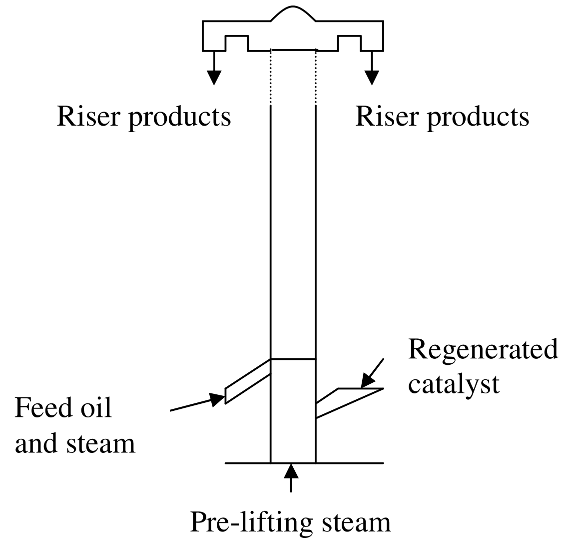

Figure 2: The FCC riser reactor

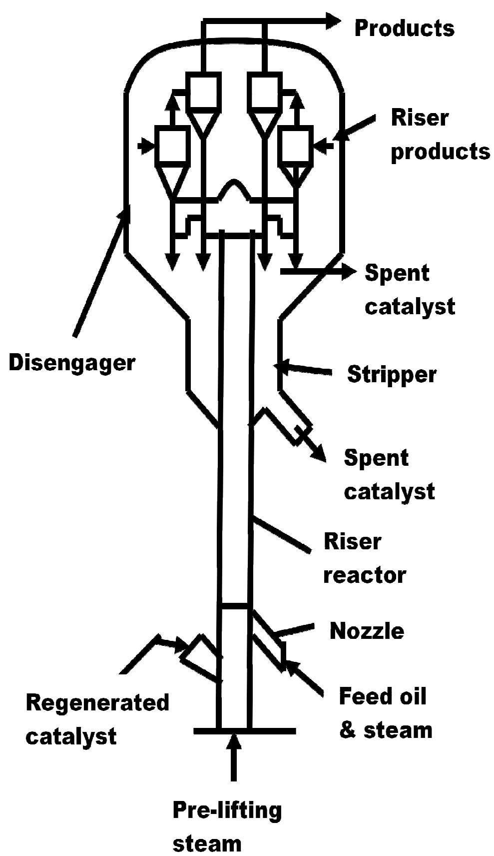

Figure 1: The FCC reactor

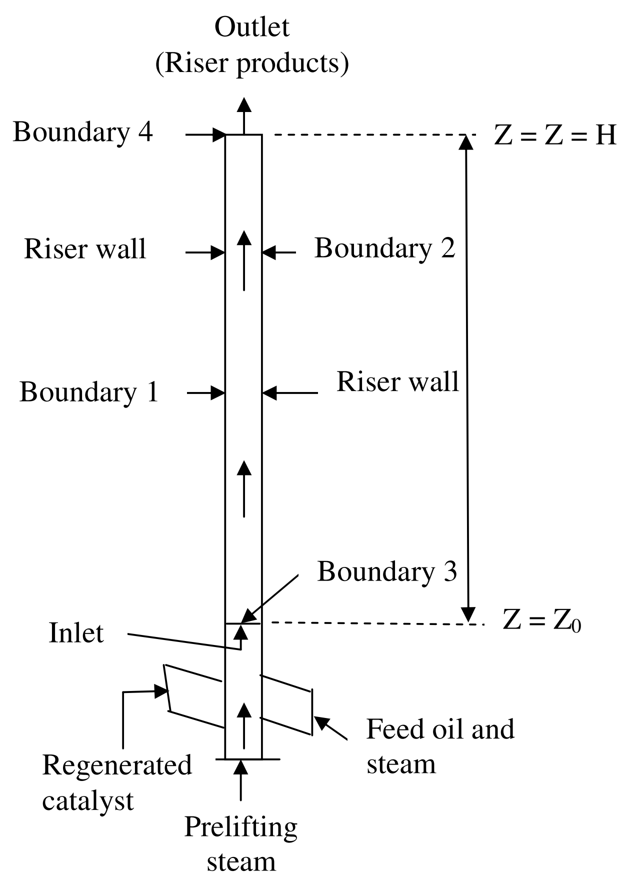

Figure 3: The FCC riser reactor without termination device simulated

Table 1
The 20 lumps of Pseudo Components

L1 = Vacuum residue	L11 = LPG
L2 = Gas oil/HFO	L12 = LPG
L3 = LFO	L13 = n-C_5 in LPG
L4 = LFO	L14 = i-C_5 in LPG
L5 = Gasoline	L15 = n-C_4 in LPG
L6 = Gasoline	L16 = i-C_4 in LPG
L7 = LPG	L17 = C_3 in LPG
L8 = LPG	L18 = C_2 = Dry Gas
L9 = LPG	L19 = C_1 =Dry Gas
L10 = LPG	L20 = C = Coke

B. The riser reactor equations

In addition to the kinetic equations the the reactor model equations as explained in [14] were used to describe the riser system. The 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).

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

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

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

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 [[9], [2], [13] as shown in equation (9) and (10) respectively.

$$r_f = aK_j C_i$$
$$j = 1,2,3,4,5,6,7,8,13,14,15 \quad (4)$$

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

$$r_f = bK_j C_i$$
$$j = 9,10,11,12,16,17,18,19,20 \quad (6)$$

$$C_c = 2.43 \times 10^{-3} t_c^{\,0.2} \quad (7)$$

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

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

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

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 choosing the void fraction variable, assumed gas velocity, slip factor and the vapourisation heat of the feed in the riser inlet are shown in [9], [13].

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

$$v = \frac{R_g T}{p} \Sigma F_i \quad (12)$$

$$p = R_g T \sum C_i \quad (13)$$

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

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

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

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.

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

$$Q = -\sum_j H_j r_j \quad (17)$$

At $z = z_0 = 0$, $w_s = 0$, $Q_{ext} = 0$, equation (16) and (17) becomes $\sum_i M_i C_{p,i} \frac{dT}{dV} - Q = 0$

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

$$T_0 = \frac{T1}{T2} \quad (18)$$

Where

T1= $(M_{cat}Cp_{cat}T_{cat}) - (M_{GO}Cpl_{GO}(T_{vap} - T_{GO}))$
$+ (M_{GO}Cpv_{GO}T_{vap}) - (M_{GO}\Delta H_{vap}) - (M_{ds}Cp_{ds}T_{ds})$

T2= $M_{cat}Cp_{cat} + M_{GO}Cpv_{GO} + M_{ds}Cp_{ds}$

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

$T_z - T_0 = -\frac{\sum_j H_j r_j}{\sum_i M_i C p_i} dv = -\frac{\sum_j H_j r_j}{\sum_i M_i C p_i} (\pi D)(z - z_0)$

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

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

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

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

C. Boundary conditions

The boundary conditions for the riser reactor are shown in table 3.

D. Materials

The average molecular weight, 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 found in [8], [9], [2]. The industrial riser reactor operating conditions are as shown in table 4.0. Plant 1 to plant 4 in table 4.0 are operating conditions adopted from [2], and Plant 5 is operating condition from [8].

III. 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 detail procedures for the simulation process is reported in [14].

IV. Result and Discussion

In plant 1, gas oil/heavy diesel oil, medium pressure steam and fresh catalyst enter the reactor riser at a temperature of 494K, 773K and 960K respectively. In plant 2, gas oil/heavy diesel oil, medium pressure steam and fresh catalyst enter the reactor riser at a temperature of 494K, 773K and 1033K respectively. In plant 3, gas oil/heavy diesel oil, medium pressure steam and fresh catalyst enter the reactor riser at a temperature of 494K, 773K and 1004K respectively. In plant 4, gas oil/heavy diesel oil, medium pressure steam and fresh catalyst enter the reactor riser at a temperature of 494K, 773K and 1006K respectively. In plant 5 (PHRC plant), gas oil/heavy diesel oil, medium pressure steam and fresh catalyst enter the reactor riser at a temperature of 505K, 464K and 1004K respectively. In all the plants, the medium pressure steam atomises the gas oil/heavy diesel oil as they travel up along the reactor riser increasing catalysis and the rate of reaction. The hydrocarbons and catalyst mixture travel upwards and the temperature inside the FCC riser decreases because of the endothermic cracking reactions. The mixture temperature at the inlet of the riser falls sharply to 794K for plant 1, 828.2K for plant 2, 793.5K for plant 3, 806.6K for plant 4 and 803 for PHRC plant because sensible heat of catalyst coming from the regenerator is utilized in providing heat for raising the sensible heat of feed, for vapourising the feed, and for further heating of the vapourised feed. Figure 4.0 shows that the mixture temperature at the inlet of the riser is 819K and the outlet temperature is 803K. The outlet temperatures from the riser for plant 1 to plant 5 are shown in table 5.0 to table 9.0. The predicted values of gasoline and coke which were compared with practical values from plant 1 to 5 are also presented in table 5.0 to 9.0. The deviation of the predicted values from plant 1 practical values is 6.62%, 1.17% and -1K for gasoline, coke and outlet temperature from the riser respectively. In the case of plant 2, the deviation is 3.6%, 1.66% and 20K for gasoline, coke and outlet temperature from the riser respectively. The deviation of the predicted values from plant 3 practical values is 7.71%, 1.57% and -11.5K for gasoline, coke and outlet temperature from the riser respectively. In the case of plant 4, the deviation is 8.72%, 1.31% and 0.6K for gasoline, coke and outlet temperature from the riser respectively while that of Plant 5, the deviation is 1.0%, 1.1% and 2K for gasoline, coke and outlet temperature from the riser respectively.

IV. V. Conclusion

The FCCU riser reactor was carefully studied and simulated using COMSOL Multiphysics software. The predicted values from the simulation were compared with operatng conditions from 5 different plants, The results show that in all cases of comparison, the deviation is minimal (±10% for gasoline and coke yields while the output temperature is ± 20k) and it is an indication that COMSOL Multiphysics software can be used to predict the yields and output temperature of the riser reactor accurately.

V. Nomenclature

The nomenclature is given in table 10 and 11

Table 2 The 20 Lumps and 190 rate constants of pseudocomponents

S/N	LUMP	CRACKED TO	RATE CONSTANTS
1.	L1	L2, L3, L4, L5, L6, L7, L8, L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{12}, K_{13}, K_{14}, K_{15}, K_{16}, K_{17}, K_{18}, K_{19}, K_{110}, K_{111}, K_{112}, K_{113}, K_{114}, K_{115}, K_{116}, K_{117}, K_{118}, K_{119}, K_{120}
2.	L2	L3, L4, L5, L6, L7, L8, L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{23}, K_{24}, K_{25}, K_{26}, K_{27}, K_{28}, K_{29}, K_{210}, K_{211}, K_{212}, K_{213}, K_{214}, K_{215}, K_{216}, K_{217}, K_{218}, K_{219}, K_{220}
3.	L3	L4, L5, L6, L7, L8, L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{34}, K_{35}, K_{36}, K_{37}, K_{38}, K_{39}, K_{310}, K_{311}, K_{312}, K_{313}, K_{314}, K_{315}, K_{316}, K_{317}, K_{318}, K_{319}, K_{320}
4.	L4	L5, L6, L7, L8, L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{45}, K_{46}, K_{47}, K_{48}, K_{49}, K_{410}, K_{411}, K_{412}, K_{413}, K_{414}, K_{415}, K_{416}, K_{417}, K_{418}, K_{419}, K_{420}
5.	L5	L6, L7, L8, L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{56}, K_{57}, K_{58}, K_{59}, K_{510}, K_{511}, K_{512}, K_{513}, K_{514}, K_{515}, K_{516}, K_{517}, K_{518}, K_{519}, K_{520}
6.	L6	L7, L8, L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{67}, K_{68}, K_{69}, K_{610}, K_{611}, K_{612}, K_{613}, K_{614}, K_{615}, K_{616}, K_{617}, K_{618}, K_{619}, K_{620}
7.	L7	L8, L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{78}, K_{79}, K_{710}, K_{711}, K_{712}, K_{713}, K_{714}, K_{715}, K_{716}, K_{717}, K_{718}, K_{719}, K_{720}
8.	L8	L9, L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{89}, K_{810}, K_{811}, K_{812}, K_{813}, K_{814}, K_{815}, K_{816}, K_{817}, K_{818}, K_{819}, K_{820}
9.	L9	L10, L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{910}, K_{911}, K_{912}, K_{913}, K_{914}, K_{915}, K_{916}, K_{917}, K_{918}, K_{919}, K_{920}
10.	L10	L11, L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{1011}, K_{1012}, K_{1013}, K_{1014}, K_{1015}, K_{1016}, K_{1017}, K_{1018}, K_{1019}, K_{1020}
11.	L11	L12, L13, L14, L15, L16, L17, L18, L19, L20	K_{1112}, K_{1113}, K_{1114}, K_{1115}, K_{1116}, K_{1117}, K_{1118}, K_{1119}, K_{1120}
12.	L12	L13, L14, L15, L16, L17, L18, L19	K_{1213}, K_{1214}, K_{1215}, K_{1216}, K_{1217}, K_{1218}, K_{1219}, K_{1220}
13.	L13	L14, L15, L16, L17, L18, L19,L20	K_{1314}, K_{1315}, K_{1316}, K_{1317}, K_{1318}, K_{1319}, K_{1320}
14.	L14	L15, L16, L17, L18, L19,L20	K_{1415}, K_{1416}, K_{1417}, K_{1418}, K_{1419}, K_{1420}
15.	L15	L16, L17, L18, L19,L20	K_{1516}, K_{1517}, K_{1518}, K_{1519}, K_{1520}
16.	L16	L17, L18, L19,L20	K_{1617}, K_{1618}, K_{1619}, K_{1620}
17.	L17	L18, L19,L20	K_{1718}, K_{1719}, K_{1720}
18.	L18	L19,L20	K_{1819}, K_{1820}
19.	L19	L20	K_{1920}
20.	L20	-	-

Table 3 Boundary conditions

SETT-INGS	BOUND-ARY 3	BOUND-ARY 4	BOUND-ARIES 1 and 2
Temperature			
Boundary type	Inlet	outlet	Wall
Boundary condition	Tempe-rature	Temper-ature	Thermal insulation
Value	T_0	T_n	-
Concentration			
Boundary type	Inlet	outlet	Wall
Boundary condition	Concentra-tion	Concentra-tion	Insulation/Symmetry
Value	c_{in} for all species	c_{out} for all species	-
Velocity and pressure			
Boundary type	Inlet	Outlet	Wall
Boundary condition	Velocity	Pressure, no viscous stress	No slip
Value	$w_0 = v_s$, $u_o = v_0 = 0$	P_0 = P-n	-

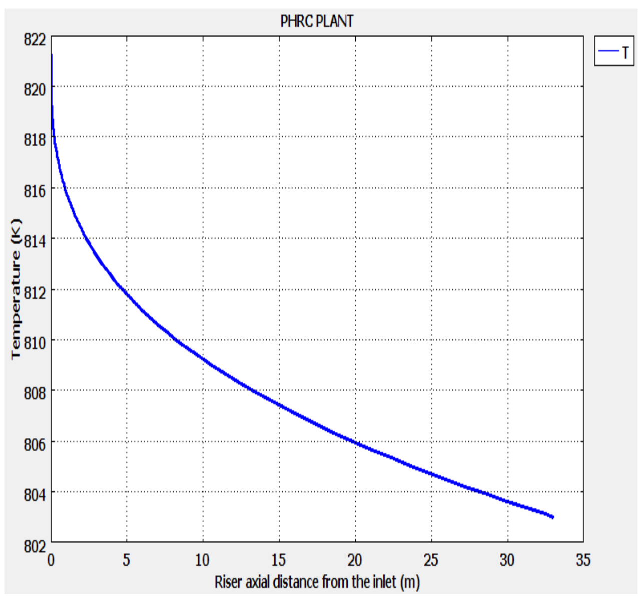

Figure 4: The temperature in the riser reactor

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Table 4: Industrial riser reactor operating conditions

Operating Conditions	Plant 1	Plant 2	Plant 3	Plant 4	Plant 5
Feed rate (kg/s)	19.95	25.7	26.9	23.6	30.87
Feed Quality (API)	22.28	21.76	22.18	22.73	D1298
COR (kg/kg)	7.2	6.33	5.43	6.07	7.04
Inlet pressure (kPa)	294	294	294	294	221
Feed temperature (K)	494	494	494	494	505
Catalyst inlet temp. (K)	960	1033	1004	1006	1004
Steam (wt%)	7	5.5	5	5.75	5
Steam temperature (K)	773	773	773	773	464

Table 5: Comparing this work with Industrial plant 1 data

yield/condition	plant 1	predicted	Deviation
Gasoline yield (wt %)	43.88	50.50	**6.62**
Coke yield (wt %)	5.83	7	**1.17**
Outlet Temp. (K)	795	794	**-1**

Table 6: Comparing this work with Industrial plant 2 data

yield/condition	plant 2	predicted	Deviation
Gasoline yield (wt %)	46.90	50.50	**3.60**
Coke yield (wt %)	5.34	7	**1.66**
Outlet Temp. (K)	808	828	**20**

Table 7: Comparing this work with Industrial plant 3 data

yield/condition	plant 3	predicted	Deviation
Gasoline yield (wt %)	42.79	50.50	**7.71**
Coke yield (wt %)	5.43	7	**1.57**
Outlet Temp. (K)	805	793.50	**-11.50**

Table 8: Comparing this work with Industrial plant 4 data

yield/condition	plant 4	predicted	Deviation
Gasoline yield (wt %)	41.78	50.50	**8.72**
Coke yield (wt %)	5.69	7	**1.31**
Outlet Temp. (K)	806	806.50	**0.60**

Table 9: Comparing this work with Industrial PHRC plant data

yield/condition	plant phrc	predicted	deviation
Gasoline yield (wt %)	49.50	50.50	**1.0**
Coke yield (wt %)	5.90	7	**1.1**
Outlet Temp. (K)	805	803	**2**

Table 10

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

Table 11

Nomenclature

(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

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