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Modelling and Simulation of an Industrial Riser in Fluid Catalytic Cracking Process

Yakubu M. John, Raj Patel, Iqbal M. Mujtaba*

Chemical Engineering Division, School of Engineering, Faculty of Engineering and Informatics, University of Bradford, Bradford, BD7 1DP, UK

*Corresponding author I.M.Mujtaba@bradford.ac.uk

Abstract

Fluid Catalytic Cracking (FCC) unit is an important unit of modern refineries and any improvement in the unit's operations and design to increase yield and meet the ever increasing demand for fuel brings about the overall profitability of the FCC. In this work, simulation of an FCC riser of varied diameter was carried out to improve the unit's operations and design, and the results are compared with risers of different diameters. The riser with varied diameter produces 53.4 wt%, a 3.18% increased yield of gasoline at low catalyst to oil (C/O) ratio of 1.27 compared to 51.7 wt% from a 1 m diameter riser. At increased C/O ratio, more gases and coke are produced in the varied diameter riser. Larger diameter demands more catalyst but yields more gases. Process variables can be directly correlated with yield of gasoline, which can aid process design.

Keywords: FCC Unit, Riser, Variable Diameter, Simulation, Modelling.

1. Introduction

The FCC unit is the workhorse of modern refineries (Bollas et al., 2007), which converts gas oil into lighter hydrocarbons used as valuable transportation fuels such as gasoline and diesel. A typical barrel of crude produces approximately 20% straight run gasoline. However, demand is nearly 50% per barrel and hence there is the need for an efficient process to increase the gasoline production. In the FCC unit, gasoline is produced in the riser and therefore it must be given considerable attention for improvement in gasoline yields.

To meet the demand for gasoline, many researchers have considered the simulation of the riser as a major strategy to improve the yield of gasoline. To do this, some important success factors like the riser design and operations must be improved. Two important factors to consider in trying to achieve optimum yield of gasoline in the riser, is to have uniform catalyst density and very effective hydrodynamics. In situations where the catalyst activity is excellent but the yield poor, the cause would be attributed primarily to the riser hydrodynamics (Kalota and Rahmim, 2003), which is a function of riser design. Therefore, riser diameter is an important factor to consider because of its effect on the riser hydrodynamics.

Although a lot of work has been carried out on the modelling of the riser, it is done by considering the riser to be of a uniform cross section (Fernandes et al., 2007, Duduku Krishnaiah, 2007, Gupta and Subba Rao, 2003, Elshishini and Elnashaie, 1990). For some, the riser comprises of a number of equal sized compartments (or volume elements) of circular cross section, but not varied diameters (Gupta et al., 2007), and for others it comprises of a cylindrical vertical vessel where cracking of gas oil is carried out using a catalyst in a vaporised upward fashion (Han and Chung, 2001a). Even when a comprehensive three-dimensional (3-D) heterogeneous riser model was applied to simulate the turbulent gas–solid flow and reaction in a polydisperse FCC riser, the entire zones of the riser were considered as a uniform cross sectional tubes (Li et al., 2013).

The riser unit has many sections; feed preheater, the vaporization section and the riser, which are sometimes modelled differently. Although an attempt to simulate the riser unit with varied diameter (between 1 m at the bottom to 1.4 m at the top) was made (Novia et al., 2007), only a quarter of the riser was considered because they modelled the riser unit in two sections; the vaporization section (found to have no chemical reactions) as 1 m diameter and the riser section as 1.4 m, a uniform cross section. They also included the vaporization section in the riser unit model. In some cases, the model of the vaporization section was included in the riser unit simulation but the length of the riser (uniform cross section) considered did not include the vaporization section (Han and Chung, 2001a, Han and Chung, 2001b). It is also clear that the vaporization section of the riser unit has unique hydrodynamics and can be treated differently, because it takes about 3% of the riser residence time (Ali and Rohani, 1997). For this reason, the riser has been modelled differently from the vaporization section with the assumption that the gas oil vaporizes instantaneously (Ahari et al., 2008, Al-Sabawi et al., 2006, Araujo-Monroy and López-Isunza, 2006). Therefore, modelling the riser unit by having different diameters for the vaporization and riser sections, is different from modelling the system where the diameter of the riser is varied. This is what this work sets to achieve; to model the riser section as a varied diameter with three different cross sections.

The riser unit of the FCC unit of Kaduna Refinery and Petrochemicals Company (KRPC) in Nigeria is a vertical cylinder but with varied diameters. This design is such that the reaction proceeds as the catalyst and vapour mixture flows up through the riser. The lower part of the riser is sized to provide sufficient pick up velocity and as cracking proceeds, the riser diameter is increased to handle the increasing volume and provide the desired reaction time. The mixture then flows through the remainder of the vertical riser.

This work modelled the riser according to geometric differences of the riser and validated against industrial data. gPROMS software is used for the simulation with C/O ratio, catalyst temperature and gas phase temperature are used as manipulating variables. The various effects of the riser geometry on the conversion of gas oil and yield of gasoline were determined.

Process Modelling

This section presents the description of the riser and its model assumptions, the model equations, degree of freedom analysis, the parameters used and method of solution of the model.

1.1 The Riser

The riser has always been modelled as a single vertical tube or cylinder but risers can have varied diameters. The riser unit of the FCC unit of KRPC is a type with varied diameters as shown in Figure 1.

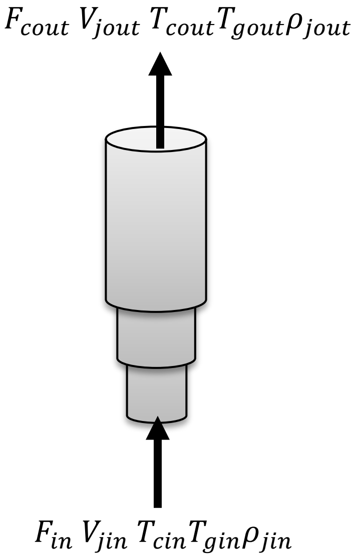


Figure 1: The Riser

It is a vertical cylinder with three different compartments, each of different diameter and height. For simplicity, the connection between each compartment is made flat as shown in Figure 1. The first compartment at the bottom has a diameter of 1.0 m and 3.965 m height. The middle compartment has a diameter of 1.35 m and 3.753 m height and the third compartment at the top has a diameter of 1.6 m and 17.6 m height. The entire height of the riser is 25.36 m. The C/O ratio of the unit varied from 2.0 to 6.5, as set by the production unit. The riser is modelled as a one-dimensional plug flow reactor without axial and radial dispersion, and mass and energy balance equations for the catalyst and gaseous phases are obtained under the following assumptions:

- the hydrocarbon feed instantly vaporizes as it comes into contact with the hot catalyst from the regenerator, then moves upwards in thermal equilibrium with the catalyst and there is no loss of heat from the riser (Ali et al., 1997).
- The cracking reactions only take place in the riser, on catalyst surface and fast enough to justify steady state model.
- The vaporization section of the riser was not considered in the simulation.
- The momentum equations of the system were not included in the simulation.
- The rate of dispersion and adsorption inside the catalyst particles are negligible.
- The coke deposited on the catalyst does not affect the velocity of the fluid.

At the entrance of the riser, the feed vaporizes immediately when it comes in contact with the regenerated catalyst and flows pneumatically upward in the riser as cracking reactions goes on the surface of the catalyst to form products. The products in this case are gasoline, gases and coke based on the four lumped model. The four lumped model to represent the kinetic model which determines the weight fractions of components in product stream as well as the reactants involved in the riser was obtained from the literature (Lee et al., 1989) and presented in Figure 2. The relevant information related to Figure 2 are presented in Table 1.

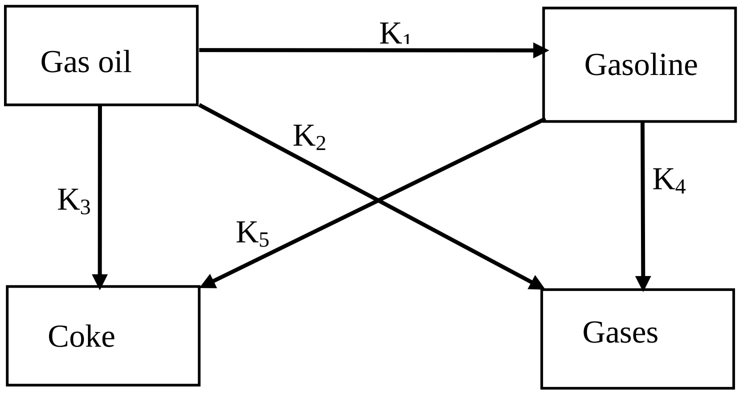


Figure 2**:** Four-lumped model of gas oil cracking reactions (Lee et al., 1989).

The formulation of a kinetic model that includes all chemical reactions responsible for the catalytic cracking of gas oil is extremely difficult and therefore, most researchers group the components into lumps to make it easier to account for the various valuable petroleum fractions. The kinetic model shown in Figure 2 is the breaking down of gas oil into gases, coke and gasoline. It is the most acceptable and widely used for its accuracy in consolidating the very important refinery fractions. The cracking reaction is endothermic and the heat required for endothermic gas oil cracking is supplied from the regenerator by burning coke formed during catalyst deactivation in the riser. Thus, accurate prediction of the coke formed due to catalyst deactivation is crucial. The coke formed aids heat integration and reactor temperature control which is one of the advantages of the four-lump model (Han and Chung, 2001a).

In Figure 2, K_1, K_2, K_3, K_4 and K_5 are the overall rate constants for the cracking reactions while their kinetic parameters are shown in Table 1. The cracking of gas oil to form gasoline, gases and coke is considered to be a second order reaction, while the cracking of gasoline to form gases and coke is considered a first order reaction.

Table 1: Kinetic parameters for gas oil cracking (Han and Chung, 2001b)

4-lump cracking reactions	Frequency factor (s^{-1})	Activation Energy (kJ/kg mol)	Heat of reaction (kJ/kg)	Reaction Path	Order of reaction
Gas oil – Gasoline	1457.50	57,359	195	1	2
Gas oil –C_1-C_4 gases	127.59	52,754	670	2	2
Gas oil- Coke	1.98	31,820	745	3	2
Gasoline–C_1-C_4 gases	256.81	65,733	530	4	1
Gasoline- Coke	$6.29\text{x}10^{-4}$	66,570	690	5	1
Catalyst deactivation	1.1x10-5	49,000			

1.2 The Model Equations

The riser shown in Figure 1 is modelled as a one-dimensional tubular reactor using mass and energy balance equations. The riser composition varies along its length, and because there is reaction going on in the riser, the dependent variables were deduced from the energy and material balance carried out on a differential element of volume as shown in Figure 3. Equations 1 and 2 are deduced temperatures of catalyst and gases respectively. Figure 3 shows the inlet and outlet compositions of the control volume.

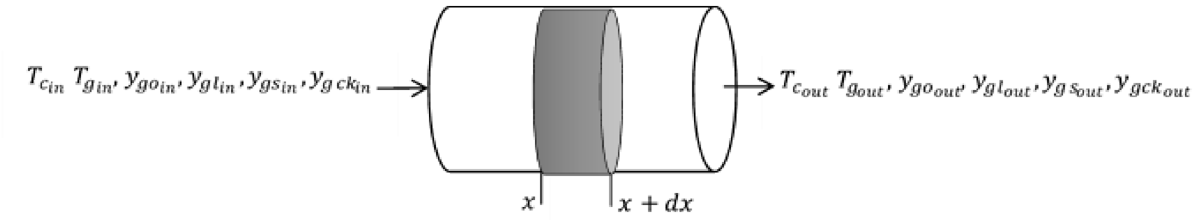


Figure 3**:** A control volume of the riser

$$\frac{dT_c}{dx} = \frac{\Omega h_p A_p}{F_c C_{pc}} (T_g - T_c) \tag{1}$$

$$\frac{dT_g}{dx} = \frac{\Omega}{F_g C_{pg}} \left[h_p A_p \left(T_c - T_g\right) + \rho_c \varepsilon_c Q_{react}\right] \tag{2}$$

Equations 3 – 6 are deduced mass fractions of gas oil, gasoline, gases and coke respectively from the mass balance carried out on the control volume of the riser:

$$\frac{d_{y_{go}}}{dx} = \frac{\rho_c \varepsilon_c \Omega \emptyset_c}{F_g} R_{go} \tag{3}$$

$$\frac{d_{y_{gl}}}{dx} = \frac{\rho_c \varepsilon_c \Omega \emptyset_c}{F_g} R_{gl} \tag{4}$$

$$\frac{d_{y_{gs}}}{dx} = \frac{\rho_c \varepsilon_c \Omega \emptyset_c}{F_g} R_{gs} \tag{5}$$

$$\frac{d_{y_{ck}}}{dx} = \frac{\rho_c \varepsilon_c \Omega}{F_g} R_{ck} \tag{6}$$

The rates of reaction for gas oil R_{go}, gasoline R_{gl}, light gas R_{gs}, and coke R_{ck}, are given as

$$R_{go} = -(K_1 + K_2 + K_3) {y_{go}}^2 \tag{7}$$

$$R_{gl} = \left(K_1 {y_{go}}^2 - K_4 y_{gl} - K_5 y_{gl}\right) \tag{8}$$

$$R_{gs} = \left(K_2 {y_{go}}^2 - K_4 y_{gl}\right) \tag{9}$$

$$R_{ck} = \left(K_3 {y_{go}}^2 - K_5 y_{gl}\right) \tag{10}$$

The rate constants K_i, of reaction path i = 1,…, 5 and their corresponding frequency factors k_{i0} are given as:

$$K_1 = k_{10} \exp\left(\frac{-E_1}{RT_g}\right) \tag{11}$$

$$K_2 = k_{20} \exp\left(\frac{-E_2}{RT_g}\right) \tag{12}$$

$$K_3 = k_{30} \exp\left(\frac{-E_3}{RT_g}\right) \tag{13}$$

$$K_4 = k_{40} \exp\left(\frac{-E_4}{RT_g}\right) \tag{14}$$

$$k_5 = K_{50} \exp\left(\frac{-E_5}{RT_g}\right) \tag{15}$$

Q_{react} is the rate of heat generation or heat removal by reaction and can be written as

$$Q_{react} = -\left(\Delta H_1 K_1 {y_{go}}^2 + \Delta H_2 K_2 {y_{go}}^2 + \Delta H_3 K_3 {y_{go}}^2 + \Delta H_4 K_4 y_{gl} + \Delta H_5 K_5 y_{gl}\right)\emptyset_c \tag{16}$$

Where the gas volume fraction, ε_g, and catalyst volume fraction, ε_c, can be obtained from:

$$\varepsilon_g = 1 - \varepsilon_c \tag{17}$$

The catalyst volume fraction, ε_c, can be written as

$$\varepsilon_c = \frac{F_c}{v_c \rho_c \Omega} \quad (18)$$

Cross sectional area of the riser, Ω, is given as

$$\Omega = \frac{\pi D^2}{4} \quad (19)$$

Effective interface heat transfer area per unit volume between the catalyst and gas phases, A_{ptc} is derived as:

$$A_{ptc} = \frac{6}{0.72 d_c} * (1 - \varepsilon_g) \quad (20)$$

The catalyst deactivation is given by:

$$\emptyset_c = \exp(-\alpha_c C_{ck}) \quad (21)$$

Where;

$$\alpha_c = \alpha_{c0} \exp\left(\frac{-E_{1c}}{RT_g}\right) (R_{AN})^{\alpha_{c*}} \quad (22)$$

and

$$C_{ck} = C_{ckCL1} + \frac{F_g y_{ck}}{F_c} \quad (23)$$

The density of the gas phase is given by:

$$\rho_g = \frac{F_g}{\varepsilon_g v_g \Omega} \quad (24)$$

The riser pressure is given by:

$$P = \rho_g \frac{RT_g}{M_{wg}} \quad (25)$$

The ratio of the mass flowrate of catalyst to the mass flowrate of gas oil is the C/O ratio and it is given by:

$$\mathrm{C/O\ ratio} = \frac{F_c}{F_g} \quad (26)$$

1.3 Degree of Freedom Analysis

The model equations are made up of six (6) ordinary differential equations (ODEs) and twenty (20) algebraic equations (AEs), making a total of twenty six (26) equations. The riser model contains thirty four (34) unknown variables as shown in Table 2. Therefore, the model is found to have 8 degrees of freedom which are specified in Table 3.

Table 2: Unknown variables in the riser model equations

Variable type	Symbol	No. of Unknown variables
Temperature	T	4
Pressure and Flowrate	P	4
Weight fraction and density	y_i, ρ	5
Heat rate	Q, A_{ptc}	2
Area and volume fraction	Ω, ε	3
Reaction coefficient	$K_i, R_i, \emptyset_c, \alpha_c, \Delta H$	16
Total of unknown variables		34

There is eight degree of freedom for the model equations and they are presented in Table 3. The first six variables in Table 3 are boundary conditions at x = 0, the entrance of the riser.

Table 3: Variables to satisfy degree of freedom

Variable	Value
y_{go} (Weight fraction of gas-oil)	1
y_{gl} (Weight fraction of gasoline)	0
y_{gs} (Weight fraction of gases)	0
y_{ck} (Weight fraction of gas-oil)	0
T_g (Temperature of gas oil, K)	513
T_c (Temperature of catalyst, K)	933
Fc (Catalyst mass flowrate, kg/s)	44.91
Fg (Gas oil mass flowrate, kg/s)	35.36

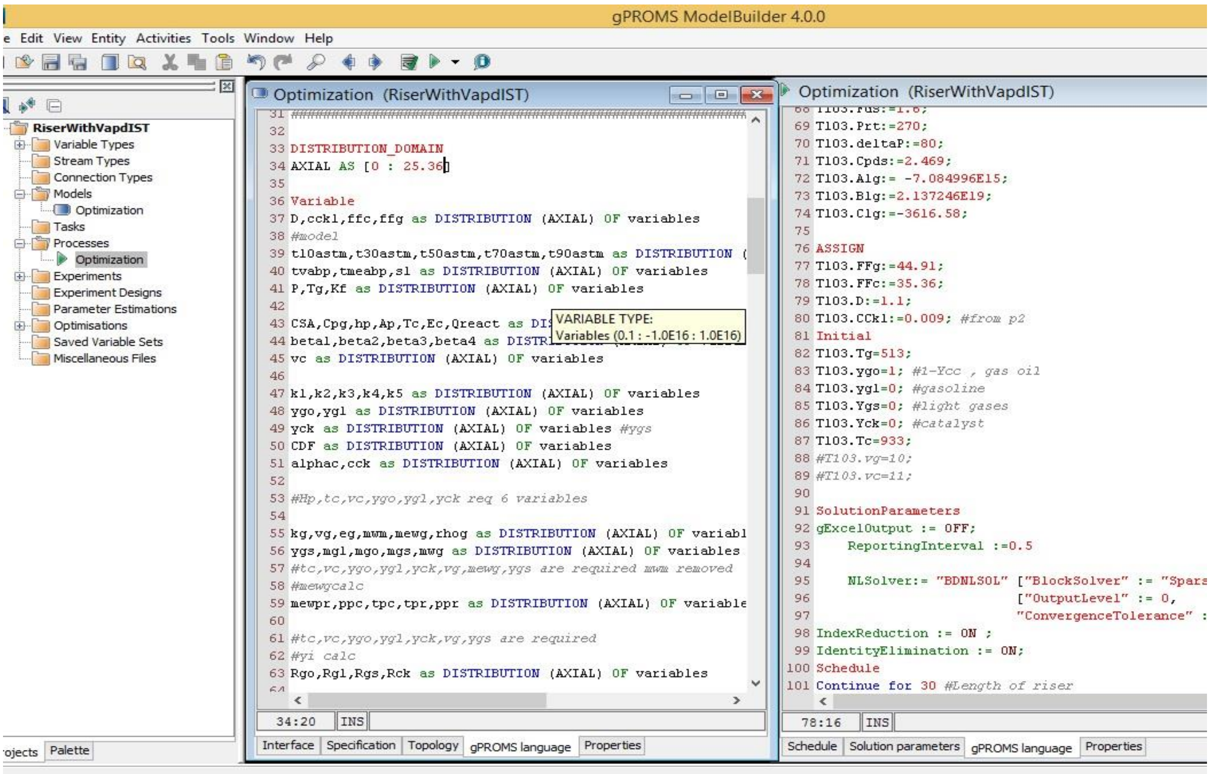
Table 4 summarizes the parameters used in this simulation and were obtained from industry and literature.

Table 4: Riser inputs parameters (Han and Chung, 2001b, Nuhu et al., 2012, Ahari et al., 2008)

Variable	Value
D (Diameter, m)	1.0, 1.35, 1.6
Riser Length (m)	25.368
T10, T30, T50, T70, T90 (TBP distillation temp at distilled vol%, ^oC)	351, 380, 409, 445, 490
M_{wgo} (Molecular weight gas oil)	371
M_{wgl} (Molecular weight gasoline)	106.7
M_{wgs} (Molecular weight light gases)	40
M_{wck} (Molecular weight coke)	14.4
D_c (Average particle diameter, m)	0.00007
S_c (Average sphericity of catalyst particles)	0.72
S_g (Specific gravity)	0.897
R_{AN} (Aromatics to Naphthenes ratio in liquid feedstock)	2.1
C_{ckc} (Coke on catalyst, kg coke/kg catalyst)	0.001
α_{c0} (pre-exponential factor of α_c)	$1.1*10^{-5}$
α_{cs} (Catalyst deactivation coefficient)	0.1177
C_{pg} (Heat capacity of Gasoline, kJ/kg K)	3.33
C_{pc} (Heat capacity of catalyst kJ/kg K)	1.15
ρ_c (Density of catalyst, kg/m^3)	1410
P, Pressure (kPa)	250

1.4 Model Solution

The equations generated for the riser are a set of Differential Algebraic Equations (DAEs) of Index 1 and gPROMS is used to solve them. gPROMS is a general process modelling system for simulation, optimisation and control (both steady state and dynamic) of highly complex processes such as the FCC unit. It is one of the available equation oriented software suitable for the type of equations developed for the riser of FCC unit. All solvers have been designed specifically for large-scale systems and there are no limits regarding problem size other than those imposed by available machine memory (Mujtaba, 2012). In spite of the robustness of gPROMS, there is no known literature of the use of the software to solve the models of the FCC unit. This is the first attempt and gPROMS proves to be a reliable software. The riser model is constructed in the model section and the parameters are specified in the process section of the gPROMS software 4.0.1. as shown in Figure 4. The distributed domain is defined in the ‘MODEL’ section as ‘DISTRIBUTION DOMAIN’ under which the distributed variables are defined as DISTRIBUTION (AXIAL) as seen in Figure 4. The boundary conditions are specified in the ‘PROCESS’ section under the ‘ASSIGN’ subsection, while the other parameters are specified in the ‘SET’ section. The gPROMS software is capable of analysing the set of equations to determine the stiffness of the system and calls on the appropriate solvers, in this case a differential-algebraic solver (DASolver) capable of solving the system of DAE of the riser model.



```
DISTRIBUTION_DOMAIN
AXIAL AS [0 : 25.36]

Variable
D,cckl,ffc,ffg as DISTRIBUTION (AXIAL) OF variables
#model
t10astm,t30astm,t50astm,t70astm,t90astm as DISTRIBUTION (
tvabp,tmeabp,sl as DISTRIBUTION (AXIAL) OF variables
P,Tg,Kf as DISTRIBUTION (AXIAL) OF variables

CSA,Cpg,hp,Ap,Tc,Ec,Qreact as DI
beta1,beta2,beta3,beta4 as DISTRI
vc as DISTRIBUTION (AXIAL) OF variables

k1,k2,k3,k4,k5 as DISTRIBUTION (AXIAL) OF variables
ygo,ygl as DISTRIBUTION (AXIAL) OF variables
yck as DISTRIBUTION (AXIAL) OF variables #ygs
CDF as DISTRIBUTION (AXIAL) OF variables
alphac,cck as DISTRIBUTION (AXIAL) OF variables

#Hp,tc,vc,ygo,ygl,yck req 6 variables

kg,vg,eg,mwm,mewg,rhog as DISTRIBUTION (AXIAL) OF variabl
ygs,mgl,mgo,mgs,mwg as DISTRIBUTION (AXIAL) OF variables
#tc,vc,ygo,ygl,yck,vg,mewg,ygs are required mwm removed
#mewgcalc
mewpr,ppc,tpc,tpr,ppr as DISTRIBUTION (AXIAL) OF variable

#tc,vc,ygo,ygl,yck,vg,ygs are required
#yi calc
Rgo,Rgl,Rgs,Rck as DISTRIBUTION (AXIAL) OF variables
```

VARIABLE TYPE:
Variables (0.1 : -1.0E16 : 1.0E16)

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T103.Prt:=270;
T103.deltaP:=80;
T103.Cpds:=2.469;
T103.Alg:= -7.084996E15;
T103.Blg:=2.137246E19;
T103.Clg:=-3616.58;

ASSIGN
T103.FFg:=44.91;
T103.FFc:=35.36;
T103.D:=1.1;
T103.CCkl:=0.009; #from p2
Initial
T103.Tg=513;
T103.ygo=1; #1-Ycc , gas oil
T103.ygl=0; #gasoline
T103.Ygs=0; #light gases
T103.Yck=0; #catalyst
T103.Tc=933;
#T103.vg=10;
#T103.vc=11;

SolutionParameters
gExcelOutput := OFF;
    ReportingInterval :=0.5

    NLSolver:= "BDNLSOL" ["BlockSolver" := "Spars
                         ["OutputLevel" := 0,
                         "ConvergenceTolerance" :
IndexReduction := ON ;
IdentityElimination := ON;
Schedule
Continue for 30 #Length of riser
```

Figure 4: gPROMS platform for the riser model

2. Results and Discussions

The manipulated variables for the simulation are catalyst-to-oil ratio (C/O), gas oil inlet temperature and catalyst inlet temperature. The results obtained are presented in Figures (5-12) and Tables 5 - 9. In Table 5, the results for two different configurations were considered in the simulation; a 1 m diameter riser and a varied diameter riser. This is to enable comparison of the two configurations and to study the effect of the diameter variation on the riser column. In the first simulation run, C/O ratio of 1.27 and 2.4 were used for both 1 m diameter riser and the varied diameter riser at catalyst inlet temperature of 933 K and gas oil inlet temperature of 513 K. The results are presented in Table 5 along with Plant data for validation of the model.

Table 5: Riser outlet weight fractions and temperatures at input C/O ratio of 1.27 and 2.4

Parameter	1 m Diameter		Varied Diameter		Plant data
C/O ratio	1.27	2.4	1.27	2.4	
Temperature of Gas, T_g (K)	579.44	688.54	563.62	685.68	796
Temperature of Catalyst, T_s (K)	584.03	691.97	564.88	686.20	
Gas oil Fraction	0.197	0.065	0.122	0.028	
Gasoline fraction	0.517	0.466	0.534	0.265	0.53
Gases	0.158	0.352	0.200	0.589	0.25
Coke	0.127	0.116	0.14	0.119	0.11

In the 1 m diameter riser and at C/O ratio of 1.27, the gas oil conversion is 80.3% (0.197 wt %) producing 51.7% (0.517 wt %) yield of gasoline, 15.8% (0.158 wt %) gases and 12.7% (0.127 wt %) coke. This indicates that gasoline yield deviated from the plant value (0.53 wt %) by -2.5%, gases yield deviated from the plant value (0.25 wt %) by -58.22% and coke yield deviated from the plant value (0.11 wt %) by 13.38%. There is a decrease in the yield of gases compared with the plant value, which is better for a case where gasoline is the desired product and needs to be improved to meet market demand. However, in this case it did not result in higher gasoline yield but produced more coke when compared with plant data. The gas phase exit temperature is not expected to be more than 800 K, beyond which most of the gasoline will be converted in a secondary reaction to gases. In this case, the temperature is 579.44 K, which is much lower than the plant exit temperature and it is the reason for the low yield of gases.

At C/O ratio of 2.4 for the same 1 m diameter riser, the gas oil conversion is 93.5% (0.065 wt %) producing 46.6% (0.466 wt %) yield of gasoline, 35.2% (0.352 wt %) gases and 11.6% (0.116 wt %) coke. This indicates that gasoline yield deviated from the plant value (0.53 wt %) by -13.73%, gases yield deviated from the plant value (0.25 wt %) by 28.98% and coke yield deviated from the plant value (0.11 wt %) by 5.17%. It shows an increase in the yield of gases compared with the plant value, and resulted in lower gasoline yield compared to plant value due to secondary reactions of gasoline to form gases and coke. The gas phase exit temperature is 688.54 K, which is lower than the plant exit temperature.

Comparing the results obtained at C/O ratio of 1.27 and C/O ratio of 2.4 for 1 m diameter riser, it is clearly seen that the gas phase temperature of 688.54 K at C/O ratio of 2.4 is higher than 579.44 K at C/O ratio of 1.27 which explains why the gasoline yield at C/O ratio of 1.27 is higher due to less heat available for gasoline secondary reaction to form gases. For the same reason, the yield of gases is higher for C/O ratio of 2.4 than for C/O ratio of 1.27. In the 1 m diameter riser, the higher the C/O ratio, the lower the yield of gasoline and coke, but higher gas oil conversion and yield of gases.

Data in Table 5 also shows that in the varied diameter riser and at C/O ratio of 1.27, the gas oil conversion is 87.8% (0.122 wt %) producing 53.4% (0.534 wt %) yield of gasoline, 20.0% (0.200 wt %) gases and 14.0% (0.140 wt %) coke. Gasoline yield deviated from the plant value (0.53 wt %) by 0.749%, gases yield deviated from the plant value (0.25 wt %) by -25.0% and coke yield deviated from the plant value (0.11 wt %) by 21.43%. There is a decrease in the yield of gases compared with the plant value which, in this case gives higher gasoline yield though produced more coke when compared with plant data. The gas phase exit temperature is 563.62 K, which is lower than the plant exit temperature and the reason for the low yield of gases.

At C/O ratio of 2.4 for the same varied diameter riser, the gas oil conversion is 97.2% (0.028 wt %) producing 26.5% (0.265 wt %) yield of gasoline, 58.9% (0.589 wt %) gases and 11.9% (0.119 wt %) coke. This indicates a 100% deviation of gasoline yield from the plant value (0.53 wt %), gases yield deviated from the plant value (0.25 wt %) by 57.55% and coke yield deviated from the plant value (0.11 wt %) by 7.56%. There is an increase in the yield of gases compared with the plant value and decrease in gasoline yield compared to plant value which is due to secondary conversion of gasoline to gases and more coke. With the increase in diameter of the riser at the top, more residence time for catalyst is created, thereby increasing the secondary reaction of gasoline. The gas phase exit temperature is 685.68 K, which is lower than the plant exit temperature.

Comparing the results for C/O ratio of 1.27 and C/O ratio of 2.4 for varied diameter riser, the gas phase temperature of 685.68 K at C/O ratio of 2.4 is higher than 563.62 K at C/O ratio of 1.27 which explains why the gasoline yield at the lower C/O ratio is higher due to gasoline secondary reaction to form gases. Also, the yield of gases is higher for C/O ratio of 2.4 than for ratio of 1.27. In the varied diameter riser, it can be concluded that the higher the C/O ratio, the lower the yield of gasoline and coke, but higher gas oil conversion and yield of gases.

For both varied and 1 m diameter risers, the yield of gasoline and coke is higher at 1.27 C/O ratio than the 2.4 C/O ratio, and more yield of gases and higher gas oil conversion for C/O ratio of 2.4 than for ratio of 1.27. In conclusion, it is better to use the varied riser at C/O ratio of 1.27 and 933 K catalyst temperature, because it gives a difference of 0.749% increase of gasoline with less yield gases and coke.

Varying the inlet temperature of catalyst can affect the cracking temperature in the riser and eventually impact on the yields of the product. The catalyst temperature was increased by 20 ^{o}C, from 933 K to 953 K for both 1 m diameter and varied diameter risers. The resulting yields of the lumps are presented in Tables 6 – 8. Table 6 shows the yield of cracking lumps at 953 K and C/O ratio of 1.27 for both 1 m diameter riser and varied diameter riser along with plant data for validation.

In the 1 m diameter riser, the gas oil conversion is 82.0% (0.18 wt %) producing 52.7% (0.527 wt %) yield of gasoline, 16.9% (0.169 wt %) gases and 12.5% (0.125 wt %) coke. The yield of gasoline deviated from the plant value (0.53 wt %) by -0.57%, gases yield deviated from the plant value (0.25 wt %) by -47.92% and coke yield deviated from the plant value (0.11 wt %) by 12.00%. A decrease in the yield of gases compared with the plant value is observed, but produced more coke when compared with plant data.

Table 6: Riser outlet weight fractions and temperatures at input C/O ratio of 1.27

Parameter	1 m Diameter	Varied diameter	Plant data
C/O ratio	1.27	1.27	
Temperature of Gas, T_g (K)	587.8	572.24	796
Temperature of Catalyst, T_s (K)	591.40	573.40	
Gas oil fraction	0.180	0.109	
Gasoline fraction	0.527	0.534	0.53
Gases	0.169	0.218	0.25
Coke	0.125	0.138	0.11

For the varied diameter riser, the gas oil conversion is 89.10% (0.109 wt %) producing 53.4% (0.534 wt %) yield of gasoline, 21.8% (0.218 wt %) gases and 13.8% (0.138 wt %) coke. The yield of gasoline deviated from the plant value (0.53 wt %) by -7.49%, gases yield deviated from the plant value (0.25 wt %) by -14.67% and coke yield deviated from the plant value (0.11 wt %) by 20.29%. There is a decrease in the yield of gases compared with the plant value, but an increase in the amount of coke produced when compared with plant data. At catalyst inlet temperature of 953 K, the gas phase exit temperature for the 1 m diameter riser is 587.8 K, which is much lower than the plant exit temperature (796 K) of the gas phase but higher than the exit temperature (572.24 K) of the gas phase for the varied diameter riser. These exit temperatures at catalyst inlet temperature of 953 K are higher compared with the exit temperatures at catalyst inlet temperature of 933 K (see Table 5), meaning that increasing the inlet catalyst temperature has a direct influence on the riser exit temperatures and it results in higher yield of gases at higher catalyst inlet temperature. The yield of gasoline at catalyst inlet temperature of 933 K (Table 5) and 953 K (Table 6) at C/O ratio of 1.27 for the varied diameter riser remained the same (0.534 wt %), which is not the case with the 1 m diameter riser where at 953 K gasoline mass fraction is 0.527 wt % and at 933 K it is 0.517 wt %, showing an increase of gasoline yield. This shows that the increase in temperature did not affect the yield of gasoline in the varied diameter riser, but reduced the yield of coke (from 0.14 wt % at 933 K to 0.138 wt % at 953 K). For both risers (1 m diameter and varied diameter), there is more gas produced at higher temperature with lower coke yield.

Table 7 shows the yield of cracking lumps at catalyst inlet temperature of 953 K and C/O ratio of 1.84 for both 1 m diameter riser and varied diameter riser along with plant data for validation. Results at C/O ratio of 1.84 at catalyst inlet temperature of 953 K in Table 7 are compared with results at C/O ratio of 1.27 in Table 6 at the same catalyst temperature. In the 1 m diameter riser, the gas oil conversion is 90.8% (0.092 wt %) producing 51.9% (0.519 wt %) yield of gasoline, 27.1% (0.271 wt %) gases and 11.9% (0.119 wt %) coke. The yield of gasoline deviates from the plant value (0.53 wt %) by -2.11%, gases yield deviates from the plant value (0.25 wt %) by 7.75% and coke yield deviates from the plant value (0.11 wt %) by 7.56%. This shows an increase in the yield of gases compared with the plant value, but produces more coke when compared with plant data.

Table 7: Riser outlet weight fractions and temperatures at input C/O ratio of 1.84

Parameter	1 m Diameter	Varied diameter	Plant data
C/O ratio	1.84	1.84	
Temperature of Gas, T_g (K)	653.64	647.64	796
Temperature of Catalyst, T_s (K)	657.37	648.33	
Gas oil fraction	0.092	0.043	
Gasoline fraction	0.519	0.400	0.53
Gases	0.271	0.432	0.25
Coke	0.119	0.124	0.11

For the varied diameter riser, the gas oil conversion is 95.7% (0.043 wt %) producing 40.0% (0.40 wt %) yield of gasoline, 43.2% (0.432 wt %) gases and 12.4% (0.124 wt %) coke. The yield of gasoline deviates from the plant value (0.53 wt %) by -32.5%, gases yield deviates from the plant value (0.25 wt %) by -42.12% and coke yield deviates from the plant value (0.11 wt %) by 11.29%. here, there is decrease in the yield of gasoline, but produced more gases and coke when compared with plant data. The 1 m diameter riser has the better yield of gasoline than the varied diameter riser. Also, the varied diameter riser produced more gases and coke than the 1 m diameter even though the 1 m diameter riser has the higher gas phase exit temperature. Comparing the yields at C/O of 1.27 and 1.84 at catalyst inlet temperature of 953 K from Tables 6 and 7 respectively, it can be concluded that operating the varied diameter riser at C/O ratio of 1.27 gives the better yield of gasoline which is the desired product. However, less coke is produced at C/O ratio of 1.84.

Table 8 shows the yield of cracking lumps at catalyst inlet temperature of 953 K and C/O ratio of 2.4 for both 1 m diameter riser and varied diameter riser along with plant data for validation. In the 1 m diameter riser, the gas oil conversion is 94.5% (0.055 wt %) producing 43.0% (0.43 wt %) yield of gasoline, 40.0% (0.400 wt %) gases and 11.3% (0.113 wt %) coke. The yield of gasoline deviated from the plant value (0.53 wt %) by -52.49%, yield of gases deviated from the plant value (0.25 wt %) by 37.5% and coke yield deviated from the plant value (0.11 wt %) by 2.65%. There is an increase in the yield of gases compared with the plant value, giving rise to decrease in gasoline yield and produced more coke when compared with plant data.

Table 8: Riser outlet weight fractions and temperatures at input C/O ratio of 2.4

Parameter	1 m Diameter	Varied diameter	Plant data
C/O ratio	2.4	2.4	
Temperature of Gas, T_g (K)	703.18	700.82	796
Temperature of Catalyst, T_s (K)	706.15	701.26	
Gas oil fraction	0.055	0.023	
Gasoline fraction	0.430	0.210	0.53
Gases	0.400	0.657	0.25
Coke	0.113	0.116	0.11

For the varied diameter riser, the gas oil conversion is 97.3% (0.023 wt %) producing 21.0% (0.40 wt %) yield of gasoline, 65.7% (0.657 wt %) gases and 11.6% (0.116 wt %) coke. The yield of gasoline deviates from the plant value (0.53 wt %) by -152.38%, gases yield deviates from the plant value (0.25 wt %) by 61.95% and coke yield deviates from the plant value (0.11 wt %) by 5.17%. This gives a very high decrease in the yield of gasoline and high yield of gases but produced more coke when compared with plant data. The 1 m diameter riser has the better yield of gasoline than the varied diameter riser. Also, the varied riser produced more gases and coke than the 1 m diameter even though the 1 m diameter riser has the higher gas phase exit temperature. Comparing the yields at C/O of 1.27, 1.84 and 2.4 at 953 K from Tables 6, 7 and 8 respectively, it can be concluded that operating the varied diameter riser at C/O ratio of 1.27 gives the better yield of gasoline which is the desire product, however, less coke is produced at C/O ratio of 1.84 and lesser coke at the C/O ratio of 2.4. The varied riser is the better choice and C/O ratio 1.27 appears to be the best condition to operate at 953 K.

Table 9 shows the simulation results when considering four different risers; 1 m diameter riser, 1.35 m diameter riser, 1.6 m diameter riser and the varied diameter riser. These were simulated at 933 K and C/O ratio of 1.84 and results obtained from the products at the exit of the risers were compared with plant data. In the 1 m diameter riser, the gas oil conversion is 89.4% (0.106 wt %) producing 53.0% (0.53 wt %) yield of gasoline, 24.40% (0.244 wt %) gases and 12.1% (0.121 wt %) coke. The yield of gasoline did not deviate from the plant value (0.53 wt %), it is the same (0.0% deviation). The yield of gases deviates from the plant value (0.25 wt %) by -2.45% and coke yield deviates from the plant value (0.11 wt %) by 9.09%.

Table 9: Riser outlet weight fractions and temperatures at input T_s = 933 K

Parameter	1 m diameter	1.35 m diameter	1.6 m diameter	Varied diameter	Plant data
C/O ratio	1.84	1.84	1.84	1.84	
Temperature of Gas T_g (K)	641.73	636.28	633.90	634.85	796
Temperature of Cat. T_s (K)	645.88	637.42	634.50	635.66	
Gas oil fraction	0.106	0.061	0.045	0.051	
Gasoline fraction	0.530	0.470	0.410	0.440	0.53
Gases	0.244	0.342	0.412	0.380	0.25
Coke	0.121	0.127	0.129	0.128	0.11

In the 1.35 m diameter riser, the gas oil conversion is 93.9% (0.061 wt %) producing 47.0% (0.47 wt %) yield of gasoline, 34.20% (0.342 wt %) gases and 12.7% (0.127 wt %) coke. The yield of gasoline deviates from the plant value (0.53 wt %) by -12.77%, yield of gases deviates from the plant value (0.25 wt %) by 22.9% and coke yield deviates from the plant value (0.11 wt %) by 13.38%. For the 1.6 m diameter riser, the gas oil conversion is 95.5% (0.045 wt %) producing 41.0% (0.41 wt %) yield of gasoline, 41.0% (0.41 wt %) gases and 12.9% (0.129 wt %) coke. The yield of gasoline deviates from the plant value (0.53 wt %) by -29.27%, yield of gases deviates from the plant value (0.25 wt %) by 39.32% and coke yield deviates from the plant value (0.11 wt %) by 14.72%. In the varied diameter riser, the gas oil conversion is 94.9% (0.051 wt %) producing 44.0% (0.44 wt %) yield of gasoline, 38.0% (0.38 wt %) gases and 12.8% (0.128 wt %) coke. The yield of gasoline deviates from the plant value (0.53 wt %) by -20.46%, yield of gases deviates from the plant value (0.25 wt %) by 34.21% and coke yield deviates from the plant value (0.11 wt %) by 14.06%.

The gas phase exit temperature decreases with increase in diameter for risers of 1 m, 1.35 m and 1.6 m diameters. Likewise, the yield of gasoline decreases with decrease in diameter for the same risers, but yield of gases increases with increase in diameter. This is because as diameter increases, the residence time for catalyst increases causing secondary reaction for gasoline being converted into gases and coke, hence the decrease in the gas phase temperature. The trend in these risers (1 m diameter, 1.35 m diameter and 1.6 m diameter) correlates in a polynomial fashion with coefficient of determination, $R^2 = 1$ as follows:

$$\text{Yield of gasoline} = -0.1143(\text{riser diameter})^2 + 0.0971(\text{riser diameter}) + 0.5471 \quad (27)$$

$$\text{Gas phase temperature } = 10.086(\text{riser diameter})^2 - 39.273(\text{riser diameter}) + 670.92 \quad (28)$$

$$\text{Yield of coke } = -0.0152(\text{riser diameter})^2 + 0.053(\text{riser diameter}) + 0.0833 \quad (29)$$

$$\text{Yield of gases } = 0.028(\text{riser diameter}) - 0.036 \quad (30)$$

These Equations (27 – 30) are only viable for the conditions they were obtained, but can be used for the typical range of riser diameters (0.61 m to 2.13 m) (Sadeghbeigi, 2012).

The results in Table 9 show that the varied diameter riser behaves like a reactor in-between risers of diameter 1.35 m and 1.6 m. This gives rise to a gasoline yield higher than in the 1.6 m diameter riser but lower than in the 1.35 m diameter riser. In conclusion, the 1 m diameter riser catalyst inlet temperature of 933 K has the best yields for gasoline and the lowest values for gases and coke.

When gas oil comes in contact with the catalyst, it begins to crack to form cracked lumps; gasoline, gases and coke. The profiles of the products of this gas oil cracking are presented in Figure 5. The gas oil inlet temperature is 513 K, the C/O ratio is 1.27 and the inlet temperature of catalyst is 933 K. Gas oil is cracked to produces three lumps; gasoline, gases and coke.

The conversion of gas oil reaches 90 wt% at the exit of the riser and 70% of that conversion is attained at 13.3 m of the riser. The coke concentration increases logarithmically from 0 wt% at the inlet to 13.0% at the exit of the riser. The gasoline increases logarithmically from 0 wt% at the inlet of the riser to its maximum yield of 51.7 wt% in the first 14 m of the riser and then essentially levels out. At the exit of the riser, the yield is 50.0 wt%. The yield of the gases increases logarithmically from 0 wt% at the inlet of the riser to a maximum of 15.8 wt% at the exit. Being an intermediate in a series reaction of consecutive reactions, the gasoline is expected to rise to a maximum and then fall. It has reached its maximum because of the consistent yield as seen in Figure 5, and about to fall if there is any secondary reaction.

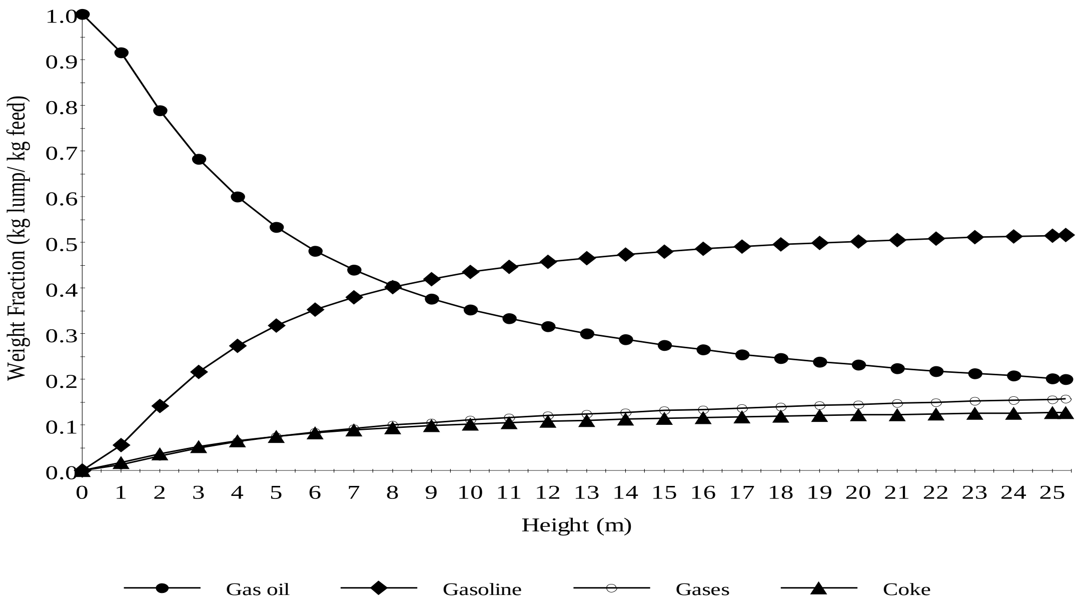

Figure 5: Weight fraction of components with 1 m diameter riser

The gasoline yield rises slightly throughout the riser and reaches to about 50 wt% at the exit of the riser which compares favorably with the value of 50 wt% obtained by Han and Chung (2001a) and 53 wt% in the plant as shown in Table 4.

The gases formed in this model logarithmically increased from 0 wt% at the inlet of the riser to 15.8 wt% at the exit of the riser as seen in Figure 3. This is expected, as the gases being a product of a multiple series–parallel reactions, should rise from a minimum to a maximum and then later levels out. The gases profile in this work compares well with that of Han and Chung (2001a). The coke composition also follows a similar logarithmic trend. However, in Figure 3, the coke is 12.7 wt% at the riser outlet for this model and it is much higher compared the plant value of 11.0 wt% shown in Table 5.

The temperature profile of both catalyst and gas phases presented in Figure 4 was obtained at the maximum C/O ratio of 2.4 which appears to have produced the lowest amount of coke deposited on catalyst at catalyst inlet temperature of 933 K and 513 K gas oil inlet temperature. The temperature of the catalyst-phase starts from about 933 K and decreases for the first 8 m and then essentially levels out. The temperature profiles of the gas phase starts from about 513 K and rises to a peak in the first 3 m of the riser and essentially levels out for the remaining portion of the riser. Both profiles approach the same value with temperature difference of about 1 K which is necessary for the completion of the reaction. The temperature profiles obtained in this work are similar to those obtained in many literatures (Han and Chung, 2001b, Souza et al., 2006, Ali et al., 1997).

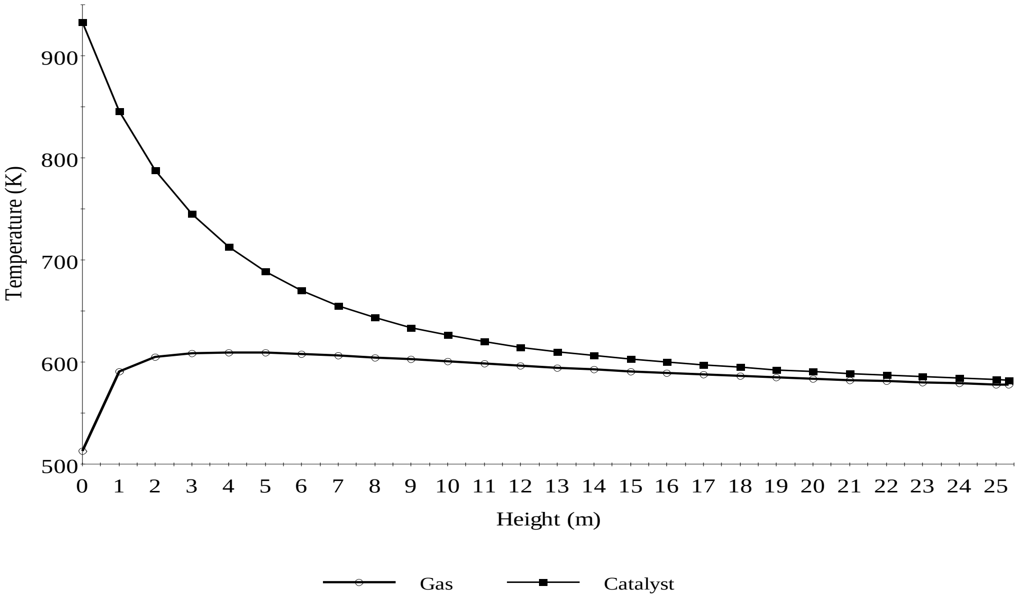

Figure 6. Temperature profile of 1 m diameter riser

The yield of coke as a lump is significant in FCC operation because of heat integration. The deactivated catalyst is regenerated by burning off the coke deposited on it and the resulting is used for the cracking of gas oil. Figure 7 compares the profiles of coke in two different risers (1 m diameter and varied diameter). The coke weight fraction profiles for both risers follows the same logarithmic trend from 0wt % at the riser entrance to 0.08 wt % at first 4 m of the riser height, then the profile for the 1 m diameter riser begin to levels out while the profile for the varied diameter riser continue to rise and eventually levels out. The exit concentrations of coke differ with more coke deposited on the catalyst for the varied diameter riser. This is possibly because of increased residence time of the catalyst in the varied diameter riser which increases the catalyst deactivation.

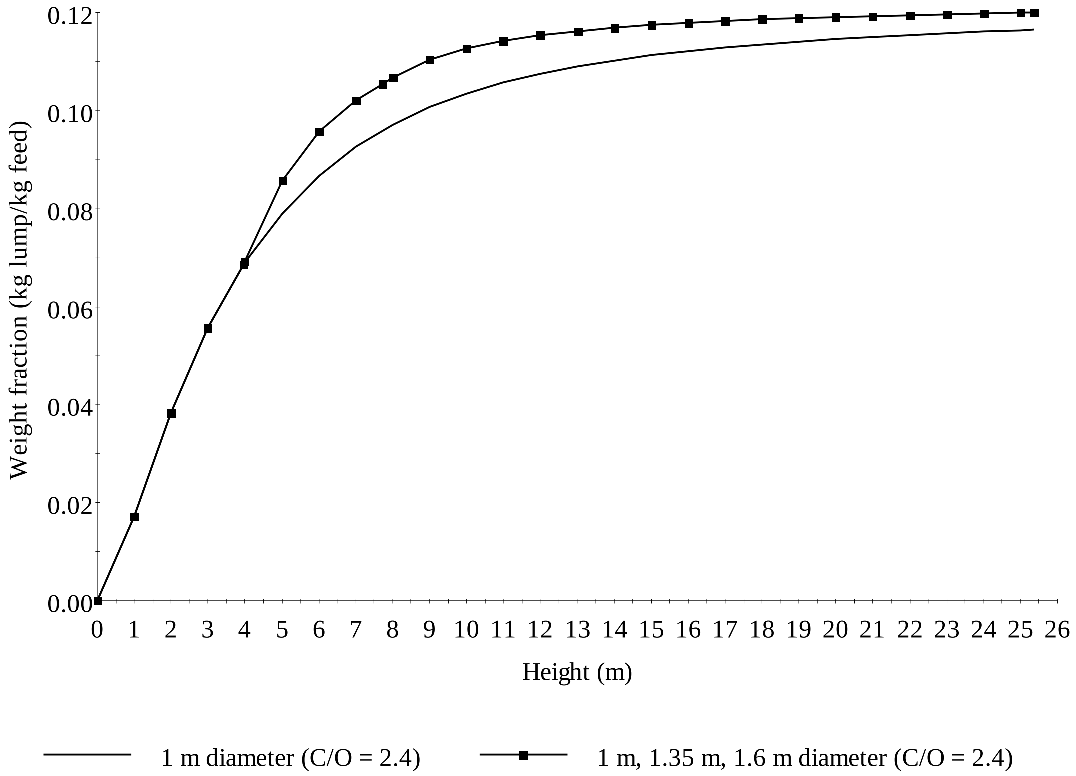

Figure 7. Weight fraction of coke in the riser at C/O ratio of 2.4 at 933 K.

Similarly, the profiles of gasoline and gases at C/O ratio of 2.4 and catalyst temperature of 933 K for 1 m diameter and varied diameter risers are presented in Figure 8.

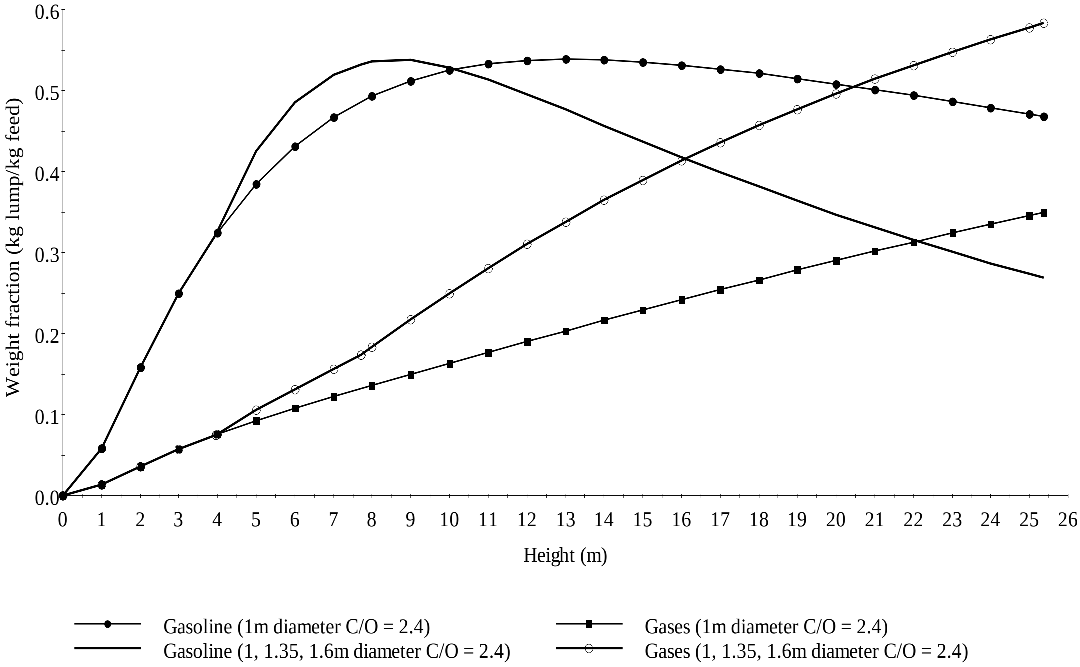

Figure 8. Weight fraction of Gasoline and Gases at C/O ratio =2.4, T_g = 933 K.

The weight fraction of gasoline rise from 0 wt % at the entrance of the 1 m diameter and the varied diameter risers and then peaking to over 50% of the yields at 10 m height of the riser then level out at the exit of the riser. However, for the varied diameter riser, the outlet weight fraction of gasoline dropped drastically compared to that of the 1 m diameter riser. This is due to increased volume of the riser as the diameter increased and consequently the residence time for catalyst increased, causing a secondary conversion of gasoline to gases, which explain why there is more gas in the varied diameter riser. This shows a trend that the C/O ratio of 2.4 favours the 1 m diameter riser because of higher gasoline yield, though it has higher coke yield too.

Four different risers (1 m diameter, 1.35 m diameter, 1.6 m diameter and varied diameter) were simulated at C/O ratio of 1.8 and catalyst temperature 933 K. The gas phase temperature profiles of the four risers are shown in Figure 9.

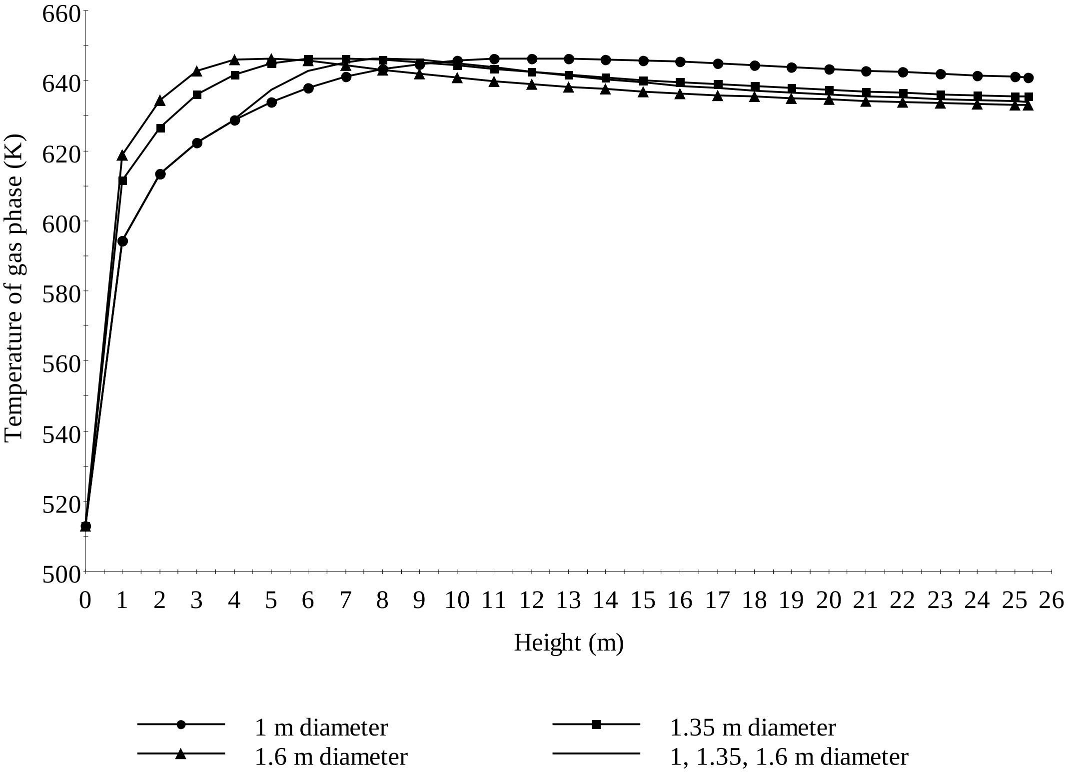

Figure 9. Temperature profiles of the four risers

The gas phase temperature profiles show great heat interactions at the inlet (first 1 m) of all the risers irrespective of the geometries. However, at the middle of the riser and towards the exit, the profile of the 1 m diameter riser shows higher temperature output due to less catalyst residence time than the catalyst residence time in the varied diameter riser. This means that the energy interactions in the riser are greatly influenced by the riser geometry. The larger the diameter of the riser, the lower is the gas phase exit temperature.

Similarly, for the four different risers the profiles of the gasoline yields are presented in Figure 10. The 1 m diameter riser produces more gasoline than the other risers, with the varied diameter riser gasoline yield slotting in-between those of risers with diameter 1.35 m and 1.6 m. Also, the 1.6 m diameter riser produced the poorest gasoline yield at this condition.

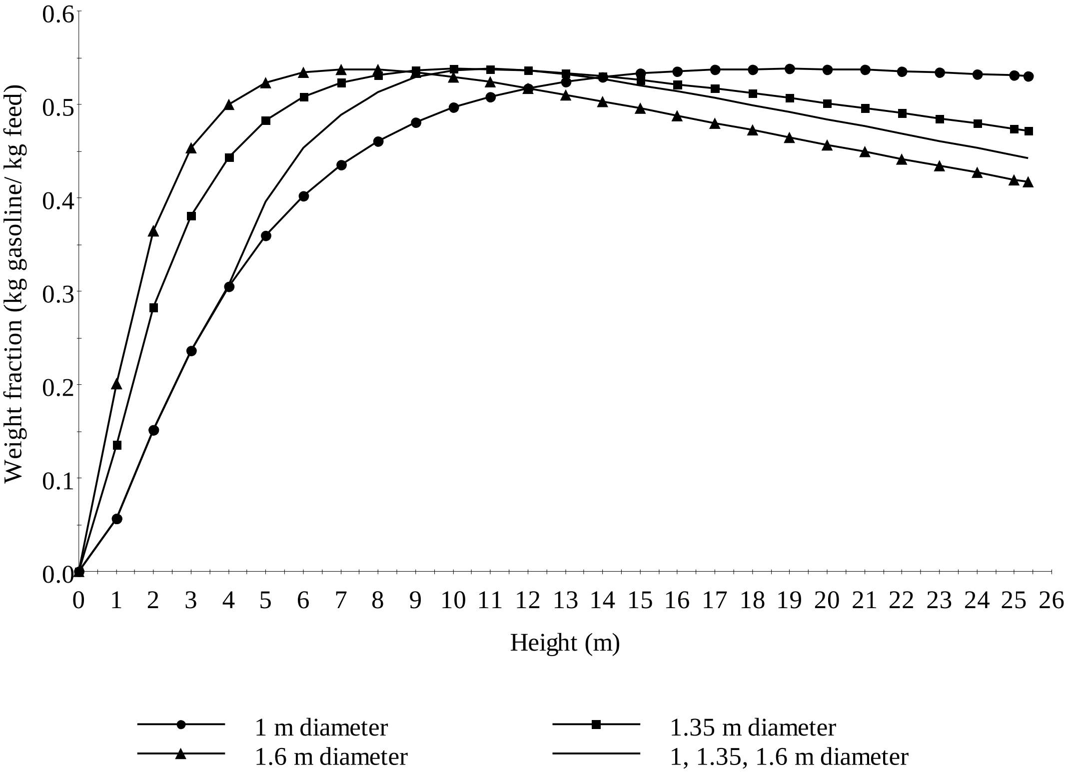

Figure 10. Gasoline yield (C/O ratio = 1.84, Tg = 513K, Ts = 933K)

The yield of gasoline at C/O ratio of 2.4 for 1 m diameter and varied diameter shown in Figure 8 and the yield of gasoline at C/O ratio of 1.84 for 1 m diameter and varied diameter shown in Figure 10 are qualitatively similar, however, quantitatively, the profiles of gasoline yields for both risers at C/O ratio 2.4 shows drastic decrease towards the exit of the risers. This is because increased C/O ratio means more catalyst is made available in the riser which favours secondary reaction of gasoline.

The temperature of catalyst was increased from 933 K to 953 K at C/O ratio of 2.4 and the profile of coke yield for 1 m diameter riser and varied diameter riser are presented in Figure

11. The coke deposited on catalyst for both risers at 953 K followed a similar qualitative trend as in coke deposited on catalyst for both risers at 933 K shown in Figure 7. The coke yield for the 1 m riser diameter is lower than in the varied diameter riser even when there is an increase of 20 ^{o}C on the catalyst temperature. In general, the higher the catalyst temperature the lower the amount of coke deposited on the catalyst.

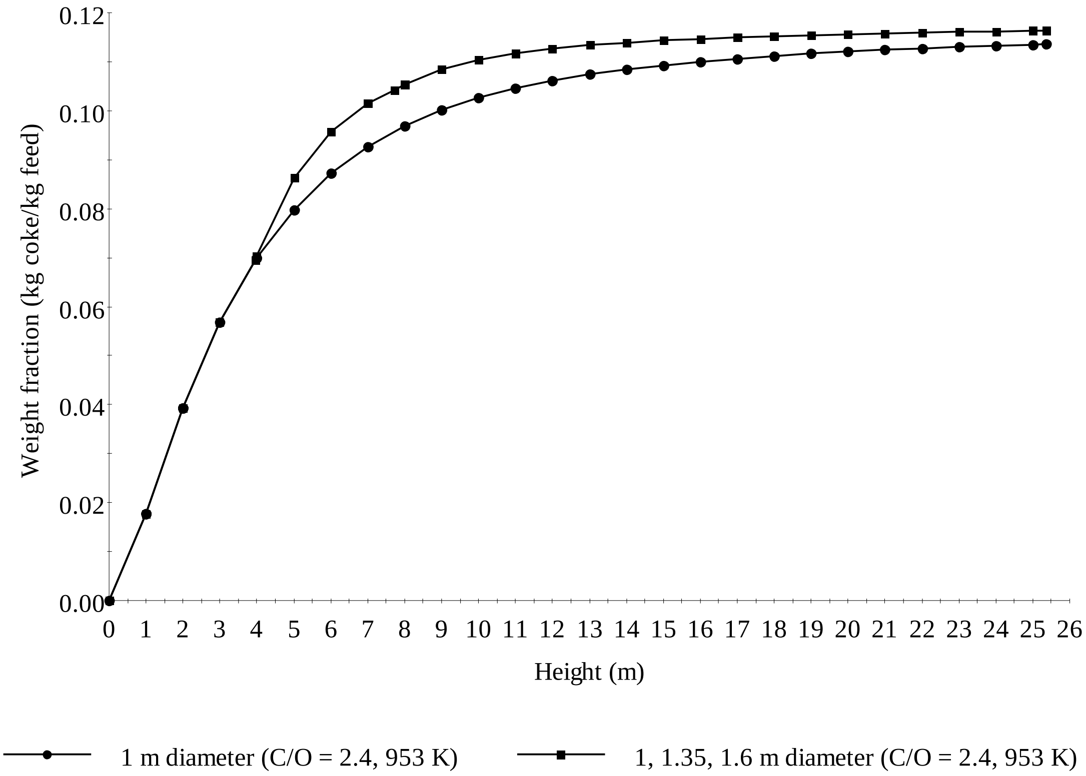

Figure 11. Weight fraction of coke at catalyst temp (953 K).

Similarly, the profiles of the weight fractions of gasoline and gases for 1 m diameter riser and varied diameter riser are presented in Figure 12 for the same conditions as those in Figure 11. The yield of gasoline and gases for both risers at 953 K followed a similar qualitative trend as in the yield of gasoline and gases for both risers at 933 K shown in Figure 8. The coke yield for the 1 m riser diameter is lower than in the varied diameter riser even when the catalyst temperature increases by 20 ^{o}C. In general, the higher the catalyst temperature the higher the yield of gases, which is an undesired product, and lower the yield of gasoline. This happens because being an endothermic reaction and more heat is injected, most of the gasoline is converted to gases.

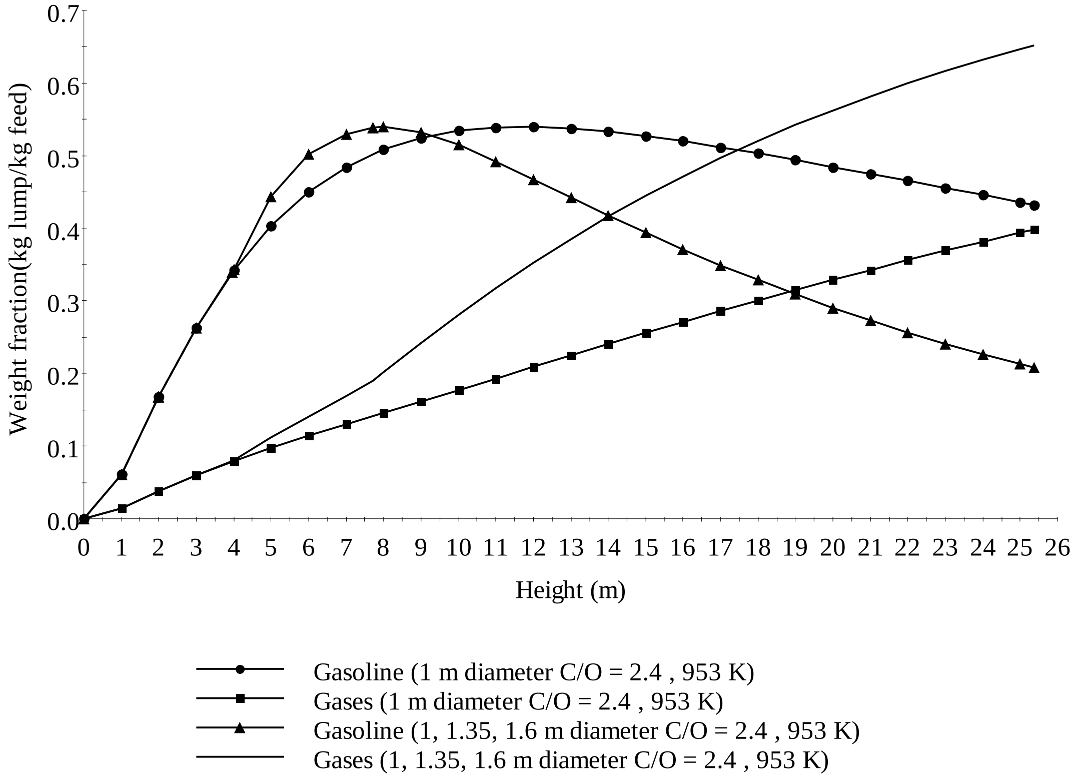

Figure 12. Weight fraction at 20 °C increase in catalyst temperature.

3. Conclusions

A varied diameter riser along with risers of uniform diameters was simulated and the following conclusions were made:

- The riser with varied diameter produces better yield of gasoline (53.4 wt %) at low catalyst to oil ratio with much closer values to plant data than that of 1 m diameter riser. At increased C/O ratio of 2.4, more gases are produced in the varied diameter riser which deviated well from the plant data and produced lower gasoline yield. This could be as a result of increased catalyst flux (Bollas et al., 2007) making more catalyst surface area available for further conversion of gasoline to gases and even coke.
- Increasing diameter of the riser, results in greater catalyst density and more heat for further cracking.
- The higher the C/O ratio and temperature, the lower the gasoline yield in all cases and the higher the yield of gases showing an inverse relationship between C/O ratio and temperature and between C/O ratio and riser diameter.

- With an increase of 20 ^{o}C catalyst temperature, gases yields increased more with increasing C/O ratio, while gasoline yield is best at the lowest C/O ratio (1.27).
- Increased diameter of the risers results in increased yield of gases.
- The riser with varied diameter behaves like the combination of all risers of different diameters. Its responses fall between the risers of diameters of 1.35 m and 1.6 m.
- With the relationship between C/O ratio, diameter and yields, refiners can easily choose the plant yield at given diameter of riser or C/O ratio.
- Further work is required which will include detail hydrodynamics of the various units of the FCC unit in relation to using a varied diameter riser and develop correlations that are applicable to all FCC models.

Notation

A	Surface area, m^2
A_{ptc}	Effective interface heat transfer area per unit volume, m^2/m^3
C	Mole concentration, kg mole/m^3
C_{p_g}	Gas heat capacity, kJ/kg K
C_{p_s}	Solid heat capacity, kJ/kg K
D	Diameter, m
d_c	Catalyst average diameter, m
E	Activation energy, kJ/kg mole
F	Mass flow rate, kg/s
H	Specific enthalpy, kJ/kg
ΔH	Heat of reaction kJ/kg
h	Enthalpy of reaction kJ/kg
h_p	Interface heat transfer coefficient between the catalyst and gas phases
h_T	Interface heat transfer coefficient, kJ/m^2 s K
k_{i0}	Frequency factor in the Arrhenius expression, 1/s
K_i	Rate coefficient of the four-lump cracking reaction, 1/s
K_g	Thermal conductivity of hydrocarbons
L	Length, m
M_w	Molecular weight
P	Pressure , kPa

Q_{react}	Rate of heat generation or heat removal by reaction, kJ/s
R	Ideal gas constant, 8.3143 kPa m^3/-kg mole K or kJ/kg mole K
RAN	Aromatics-to-naphthenes ratio in liquid feedstock
S_c	Average sphericity of catalyst particles
S_g	Total mass interchange rate between the emulsion and bubble phases, 1/s
T	Temperature, K
u	superficial velocity, m/s
V	Volume, m^3
y	Weight fraction
Zg	Gas compressibility factor

Greek

Ω	Cross-sectional area
ρ	Density, kg/m^3
$\emptyset$	Catalyst deactivation function
ε	Voidage
α	Catalyst deactivation coefficient
α_C^*	exponent for representing α
μ_g	viscosity

Subcript

cc	Coke on catalyst
ck	coke
g	Acceleration m/s^2
gl	gasoline
go	Gas oil
gs	gases
MABP	Molal average boiling temperature, K
MeABP	Mean average boiling temperature, K
pc	pseudo-critical
pr	pseudo-reduced
Rs	Riser

Appendix A

Table A.1 and Equations A1 – A24 are correlations of physical and transport parameters adopted from the literature (Han and Chung, 2001a, Han and Chung, 2001b).

Table A.1: Distillation Coefficients

Volume % distilled	a	b
10	0.5277	1.0900
30	0.7429	1.0425
50	0.8920	1.0176
70	0.8705	1.0226
90	0.9490	1.0110

Heat capacity of gas, C_{pg}, is

$$C_{pg} = \beta_1 + \beta_2 T_g + \beta_3 T_g^2 \tag{A.1}$$

Where β_1, β_2, β_3 and β_4 catalyst decay constant given as

$$\beta_1 = -1.492343 + 0.124432K_f + \beta_4\left(1.23519 - \frac{1.04025}{S_g}\right)$$

(A.2) $$\beta_2 = (-7.53624 \times 10^{-4})\left[2.9247 - (1.5524 - 0.05543K_f)K_f + \beta_4\left(6.0283 - \frac{5.0694}{S_g}\right)\right]$$

(A.3)

$$\beta_3 = (1.356523 \times 10^{-6})(1.6946 + 0.0884\beta_4) \tag{A.4}$$

$$\beta_4 = \left[\left(\frac{12.8}{Kf} - 1\right)\left(1 - \frac{10}{Kf}\right)\left(S_g - 0.885\right)\left(S_g - 0.7\right)(10^4)\right]^2 \text{ For } 10 < Kf < 12.8 \tag{A.5}$$

Else $\beta_4 = 0$ for all other cases

Kf is the Watson characterization factor written as

$$Kf = \frac{(1.8T_{MeABP})^{\frac{1}{3}}}{S_g} \tag{A.6}$$

Where M_{wg} is the molecular weight of the gas and can be calculated using

$$M_{wg} = 42.965\left[\exp\left(2.097 \times 10^{-4} T_{MeABP} - 7.787 S_g + 2.085 \times 10^{-3} T_{MeABP} S_g\right)\right] \left(T_{MeABP}^{1.26007}\ {S_g}^{4.98308}\right) \quad (A.7)$$

$$T_{MeABP} = T_{VABP} - 0.5556\exp[-0.9440 - 0.0087(1.8T_{VABP} - 491.67)^{0.6667} + 2.9972(Sl)^{0.3333} \quad (A.8)$$

Where T_{VABP} , the volume average boiling temperature and (Sl) is slope given as

$$(Sl) = 0.0125(T_{90ASTM} - T_{10ASTM}) \quad (A.9)$$

$$T_{VABP} = 0.2(T_{10ASTM+}\ T_{30ASTM+} T_{50ASTM+}\ T_{70ASTM+}\ T_{90ASTM}) \quad (A.10)$$

The ASTM D86 distillation temperatures are calculated using

$$T_{10ASTM} = a_{10}^{-\frac{1}{b_{10}}} (T_{10TBP})^{\frac{1}{b_{10}}} \quad (A.11)$$

$$T_{30ASTM} = a_{30}^{-\frac{1}{b_{30}}} (T_{30TBP})^{\frac{1}{b_{30}}} \quad (A.12)$$

$$T_{50ASTM} = a_{50}^{-\frac{1}{b_{50}}} (T_{50TBP})^{\frac{1}{b_{50}}} \quad (A.13)$$

$$T_{70ASTM} = a_{70}^{-\frac{1}{b_{70}}} (T_{70TBP})^{\frac{1}{b_{70}}} \quad (A.14)$$

$$T_{90ASTM} = a_{90}^{-\frac{1}{b_{90}}} (T_{90TBP})^{\frac{1}{b_{90}}} \quad (A.15)$$

Where a_i and b_i are distillation coefficients (Table A.1) and T_{iTBP} is the TBP distillation temperature.

Interface heat transfer coefficient between the catalyst and gas phases,h_p,

$$h_p = 0.03 \frac{K_g}{d_c^{\frac{2}{3}}} \left[\frac{|(v_g - v_c)| \rho_g \varepsilon_g}{\mu_g}\right]^{\frac{1}{3}} \quad (A.16)$$

Thermal conductivity of hydrocarbons

$$K_g = 1 \times 10^{-6}(1.9469 - 0.374M_{wm} + 1.4815 \times 10^{-3} M_{wm}^2 + 0.1028T_g) \quad (A.17)$$

M_{WM} is the mean molecular weight of the combined catalyst and gas

$$M_{WM} = \frac{1}{\left(\frac{ygo}{M_{wgo}}+\frac{ygl}{M_{wgl}}+\frac{ygs}{M_{wgs}}+\frac{yck}{M_{ck}}\right)} \quad (A.18)$$

$$M_{wgo} = M_{wg} \quad (A.19)$$

$$M_{wgs} = 0.002M_{wH_2} + 0.057M_{wC_1} + 0.078M_{wC_2} + 0.297M_{wC_3} + 0.566M_{wC_4} \quad (A.20)$$

The viscosity of the gas

$$\mu_g = 3.515 \times 10^{-8}\mu_{pr}\frac{\sqrt{M_{WM}P_{pc}^{\frac{2}{3}}}}{T_{pc}^{\frac{1}{6}}} \quad (A.21)$$

$$\mu_{pr} = 0.435 \exp\left[\left(1.3316 - T_{pr}^{0.6921}\right)P_{pr}\right] T_{pr} + 0.0155 \quad (A.22)$$

$$\begin{aligned} T_{pc} = {} & 17.1419\left[\exp\left(-9.3145 \times 10^{-4}T_{MeABP} - 0.5444S_g + 6.4791 \times 10^{-4}T_{MeABP}S_g\right)\right] \\ & \times T_{MeAB}^{-0.4844}S_g^{4.0846} \end{aligned} \quad (A.23)$$

$$\begin{aligned} P_{pc} = {} & 4.6352 \times 10^{6}\left[\exp\left(-8.505 \times 10^{-3}T_{MeABP} - 4.8014S_g + 5.749 \times 10^{-3}T_{MeABP}S_g\right)\right] \\ & \times T_{MeAB}^{-0.4844}S_g^{4.0846} \end{aligned} \quad (A.24)$$

$$T_{pr} = \frac{T_g}{T_{pc}} \quad (A.25)$$

$$P_{pr} = \frac{P}{P_{pc}} \quad (A.26)$$

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