Journal of Applied Sciences

ISSN 1812-5654

Journal of Applied Sciences 14 (23): 3172-3181, 2014
ISSN 1812-5654 / DOI: 10.3923/jas.2014.3172.3181

3D CFD Modeling and Simulation of RFCC Riser Hydrodynamics and Kinetics

Aisha Ahmed, A. Maulud, M. Ramasamy, K.K. Lau and S. Mahadzir
Department of Chemical Engineering, Universiti Teknologi PETRONAS, Tronoh, 31750, Malaysia

Abstract: The riser of an industrial RFCC unit is simulated using a steady-state multi-fluid Eulerian 3D model in ANSYS FLUENT workbench 14. The comprehensive hydrodynamics model together with 7-lump kinetic model describes the flow behavior and cracking reactions inside the riser very well. The radial variation in the axial particle velocity and particle volume fraction is found. The product distribution and temperature distribution along the riser shows very good agreement with the industrial RFCC plant data.

Key words: RFCC riser, 7-lumps, k-ε turbulence, kinetic theory, granular flow, ANSYS fluent

INTRODUCTION

Fluid Catalytic Cracking (FCC) unit plays a key role in an integrated refinery as the primary conversion process. In this process the high boiling point hydrocarbon fractions of petroleum crude oils is converted into more valuable gasoline, olefinic gases and other products by using a very active zeolite catalyst in a circulating fluidized bed (Meyers and Hunt, 2003; Sadeghbeigi, 2012). Market demands and developments in new catalysts drive the evolution of technologies for processing heavier feeds such as atmospheric or even hydro-treated vacuum residues. Residual oil Fluid Catalytic Cracking (RFCC) units charge conradson carbon residue and metal contaminated feedstocks, such as atmospheric residues or mixtures of vacuum residue and gas oils to maximize gasoline production. The hydrodynamics of FCC riser reactor has been studied with different modeling approaches. The accurate analysis of the flow field has not yet been achieved and very often, it is limited to a two-dimensional flow description because of heavy CPU time requirements.

Computer simulation of a multiphase reacting flow systems helps in understanding and analyzing the flow dynamics together with the chemical kinetics inside the riser and simultaneously solves their complex models. Many research studies have been employing the Computational Fluid Dynamics (CFD) modeling for the FCC riser and downer reactors, some of which model the two-phase reacting flow without considering turbulence and diffusion of particle phase (Theologos *et al*., 1999). Others studied the gas-particle turbulent flow with kinetic theory of granular flow without considering the kinetics model (Huilin *et al*., 2003; Almuttahar and Taghipour, 2008; Shah *et al*., 2011; Hodapp *et al*., 2012). Also Das *et al*. (2003) studied the two phase reacting flow in 3D model using the density-based solution algorithm while Lan *et al*. (2009) considered the kinetics of the 14-lumps model in a Two-Stage Riser Fluid Catalytic Cracking unit. Lopes *et al*. (2011) developed a 3D CFD simulation model with a 4-lump kinetics model and a gas-phase turbulence model for a FCC riser, neglecting the particles turbulence. None of these works model the RFCC riser.

In this study, a steady state and pressure-based 3D model for the riser of an industrial RFCC unit was developed using ANSYS FLUENT in workbench 14.0. The reacting flow in the riser is simulated incorporating the gas-solid turbulence and the particle flow kinetic theory. The 7-lump kinetic by Xu *et al*. (2006) is used to describe the catalytic cracking reactions.

RFCC RISER MODEL

In this study, the governing equations of the 3D species transport model and the k-ε turbulence model per phase together with the kinetic theory of granular flow models are solved with the following assumptions:

- Vaporization of the feed is instantaneous and the vapor and catalyst inlet temperatures are estimated at the point of contact
- Catalyst particles are spherical with average diameter and have homogeneous distribution inside the dense and dilute phases
- Inlet component concentration inside the solid phase is based on the assumption that the regenerated catalyst pores are filled with steam only

Kinetic reaction model: A 7-lump kinetic model considering all the products and coke as separate lumps

Corresponding Author: Aisha Ahmed, Department of Chemical Engineering, Universiti Teknologi PETRONAS, Tronoh, 31750, Malaysia Tel: +60125254986

proposed by Xu *et al*. (2006) is chosen in the present study. Catalyst deactivation due to coke formation make it very important to consider coke as separate lump for more accurate prediction. The reaction scheme for RFCC riser in Fig. 1 shows that there are 18 reactions taking place between the 7 lumps. An irreversible pseudo first order reaction was accepted for all reactions in this model, hence the reaction rate of a pseudo-species j is:

$$r_j = -k_j' \rho_c \frac{(\rho a_j)}{\varepsilon} \quad (1)$$

Where:

$$k_j = k_j f(C_{Arh}) \phi(t_c) f(N) \quad (2)$$

$$f(C_{Arh}) = \frac{1}{(1+K_h C_{Arh})} \quad (3)$$

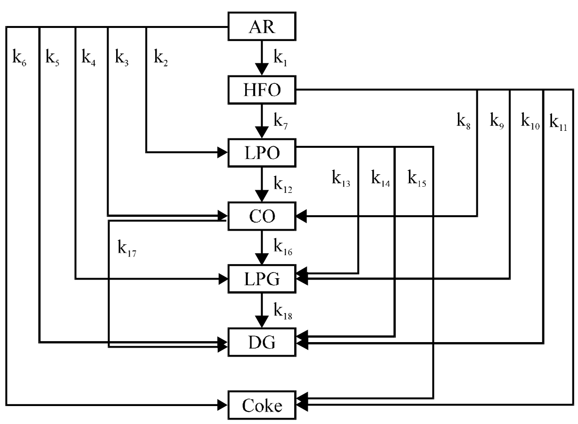

Fig. 1: A 7-lump reaction scheme for RFCC

$$\varphi(t_c) = \frac{1}{(1+\beta' t_c^{\gamma'})} \quad (4)$$

With regard to high catalyst to oil ratio, the nitrogen poisoning deactivation function f(N) can be neglected because of its insignificance. Taking the ideal gas assumption, the reaction rate can be expressed as:

$$r_j = -k_j f(C_{Arh}) \varphi(t_c) \frac{\rho_c}{\varepsilon} \frac{\rho}{M_W} Y_j \quad (5)$$

In this study, the heat of cracking reactions for each of the 18 reactions is calculated from:

$$Q_r = \Sigma(-r_j \times \Delta H_{crack}) \quad (6)$$

Where:

$$\Delta H_{crack} = \sum_1^P \left[\int_{T_o}^T \nu_j C_{P,j} dT\right] + \sum_1^P \nu_j \Delta H_{vap,j} + \Delta H^\circ - \sum_1^R \nu_j \Delta H_{vap,j} - \sum_1^R \left[\int_{T_o}^T \nu_j C_{P,j} dT\right] \quad (7)$$

$$\Delta H^\circ = \sum_1^P \nu_j \Delta H_{f,j}^\circ - \sum_1^R \nu_j \Delta H_{f,j}^\circ \quad (8)$$

The stoichiometric coefficients V_j are calculated as ratios of the average molecular weights of the lumps (Xu *et al*., 2006). Heats of formation and heats of vaporization of the species are found from (ENSPM, 1999; Pekediz *et al*., 1997). The estimated kinetic parameters by Xu *et al*. (2006) through their unit factors regression and the calculated heats of cracking reaction for the 18 stoichiometric reactions were tabulated in Table 1.

Table 1: A 7-lump model reactions, kinetic parameters and heats of reactions

R×n No.	Reaction	Frequency factor k_o (m^3/(kg cat.h))	Activation energy E (kJ $kmol^{-1}$)	$\Delta H_{cracl}\times10^{-4}$ (kJ $kmol^{-1}$)
1	AR→2.461 HFO	35520	50727	+40.213
2	AR→4.149 LFO	13750	50727	+30.136
3	AR→8.068 GO	2780	50727	+28.610
4	AR→20.34 LPG	42.68	16150	+18.336
5	AR→51.63 DG	4.268	16150	+234.777
6	AR→2.375 Coke	137.3	16150	+196.071
7	HFO→1.686 LFO	13750	16150	-4.097
8	HFO→3.277 GO	1130	46240	-4.696
9	HFO→8.265 LPG	1284	59750	+31.744
10	HFO→20.98 DG	128.4	59750	+79.060
11	HFO→0.965 Coke	3101	59750	+63.330
12	LFO→1.944 GO	686.4	46240	-0.360
13	LFO→4.904 LPG	81.22	59750	+21.257
14	LFO→12.45 DG	8.122	59750	+49.334
15	LFO→0.573 Coke	564.6	59750	+40.008
16	GO→2.523 LPG	43.66	78490	+11.119
17	GO→6.402 DG	21.83	78490	+25.559
18	LPG→2.538 DG	31.74	59750	+5.724

Table 2: Operating conditions of the industrial RFCC unit

Operating conditions	Value	Operating conditions	Value
Catalyst type (zeolite)		Reaction pressure (kPa)	361.30
Particle diameter (μm)	77	COR	6.88
Particle density (kg m^{-3})	1700	Pre-lift steam (kg sec^{-1})	2.46
Particle mass flux (kg m^{-2} sec)	320	Feed flow rate (t h^{-1})	219.17
Superficial gas velocity (m sec^{-1})	5.7	Conversion	73.79
Riser inside diameter (m)	1.36	Catalyst circulation rate (t h^{-1})	1670.00
Riser hight (m)	38	Recycle oil (%wt. of feed)	15.00
Reaction temperature (°C)	508		

Table 3: Numerical parameters

Parameters	Condition	Description
Model	Solver	3D steady-state, pressure-base
	Multiphase	Eulerian-Eulerian
	Turbulence	Standard k-ε, Standard Wall Fn, per phase
	Species	Species Transport, Reactions
KTGF parameters	Granular temp.	Partial differential equation
	Granular viscosity	Gidaspow (1994)
	Drag coefficient	Huilin *et al.* (2003)
	Interphase heat transfer	Gunn (1978)
	Particle-Particle restitution coeff	0.99
	Wall-particle restitution coeff	0.95
	Specularity	0.5
Under-relaxation factors	Pressure	0.3
	Momentum	0.2
	Volume fraction	0.4

Numerical procedure: According to the grid independence test, 468160 hexahedral elements built from the body sizing was chosen to simulate the riser. The outflow boundary condition is taken for the outlet of the riser and the inlet boundary conditions were estimated from the method of Zheng *et al.* (2001). Species properties from the refining data book (ENSPM, 1999) were fed as input to the FLUENT materials list. Other operating conditions of the industrial RFCC unit are given in Table 2 and 3 shows the modeling parameters used in the simulation.

RESULTS AND DISCUSSION

The contours of the axial solid velocity describe the fully developed flow in the riser, where same contours are observed at different levels along the riser as shown in Fig. 2a. The maximum velocity of about 24.4 m sec^{-1} at the riser axis and the average velocity at the outlet is 12.63 m sec^{-1}. After the first 10 m, the axial velocity profiles of the particle phase are almost equal as shown in Fig. 2b. Figure 3a shows the contour of particle volume fraction at the same different levels across the riser length. Also same profiles are obtained at level 19, 28 and 38 m (Fig. 3b). It is obvious from these figures that the dilute gas-particle stream flows upwards in the core of the riser and the solids mainly accumulate at the walls. Hence, the 3D simulation illustrates well the core-annular flow pattern of the solids. The particles tend to drag the gas downward in the wall region producing significant internal recirculation of both particles and gas in the riser that disappears at very high gas velocities.

In fluidized beds, including risers, the particles motion is in large scale like the random motion of clusters and there exist appreciable differences between the particle collisions and particles turbulence. Therefore, particles turbulence was considered in this model which is similar to the motion of eddies in single-phase turbulence. Figure 4a-b show that both turbulent kinetic energy and dissipation rate have very low values in the contact zone below 10 m, then increase towards the top. Maximum kinetic energy at the top of the riser is found in the annular region between centre core and wall while maximum dissipation rate is found at the wall before the top of the riser.

It has been known that the gas-solid flow behaviors in the riser and solid circulation rate are strongly dependent upon pressure drops of different sections of the RFCC unit. The overall pressure balance included in the momentum balance equations together with the conservation of granular temperature in kinetic theory of granular flow results in a maximum pressure drop of 25 kPa along the riser, as shown in Fig. 5. This agrees with the pressure drop in the riser of the industrial plant. Also reaction temperature strongly affects the products yields and reaction rate. The maximum variation of the temperature for both phases occurs near the entry zone. Since, instantaneous feed vaporization is assumed, the inlet temperatures were estimated for the gas and particle phases at the contacting zone (Berry *et al.*, 2004; Behjat *et al.*, 2011). Figure 6 illustrates the prediction of the actual temperature distribution for the solid phase along the riser. The temperature drops sharply in the centre core of the riser at the contact zone and it is high

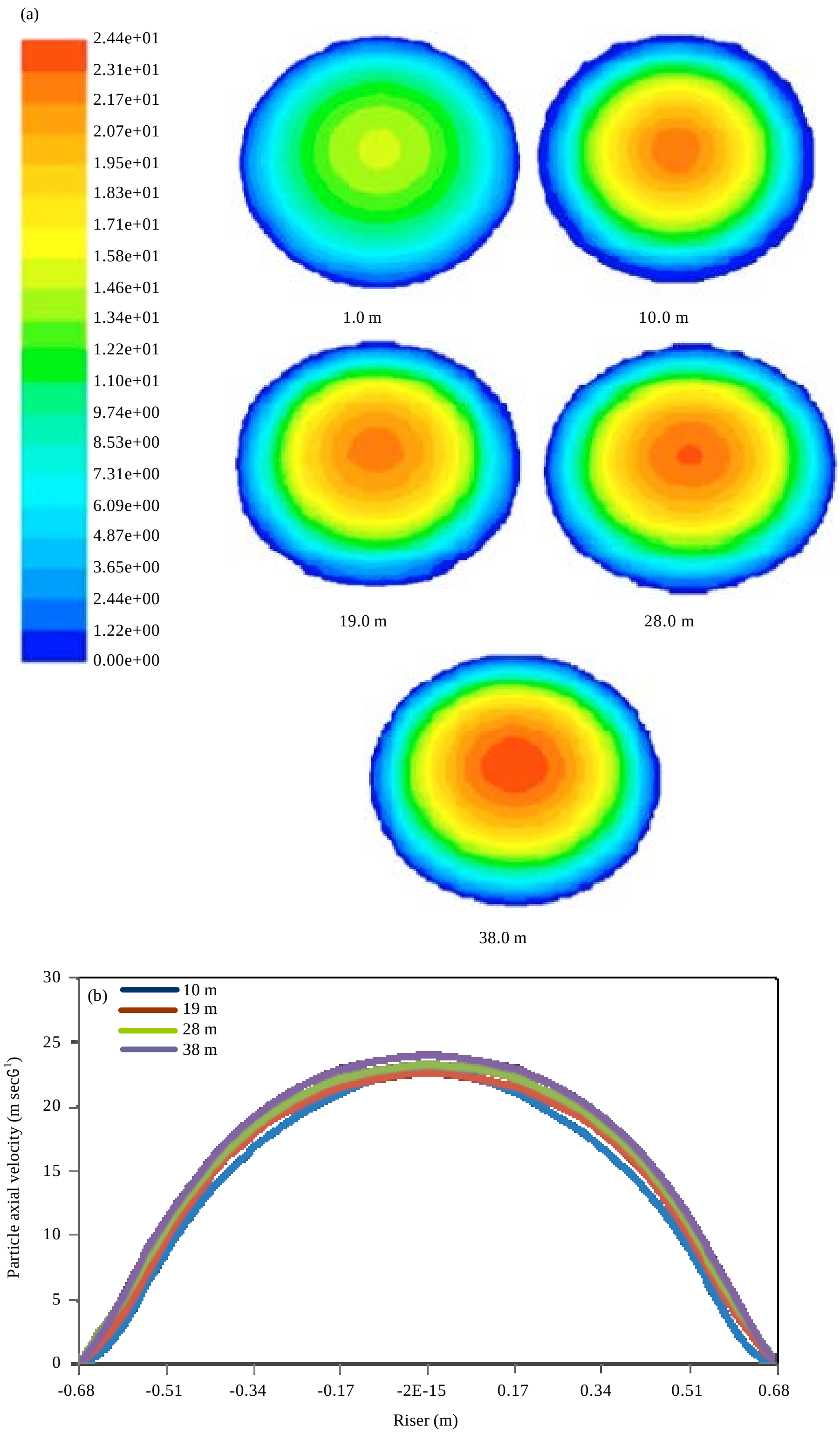

Fig. 2(a-b): Particle axial velocity on planes at different levels along the riser (a) Contour and (b) Radial profile

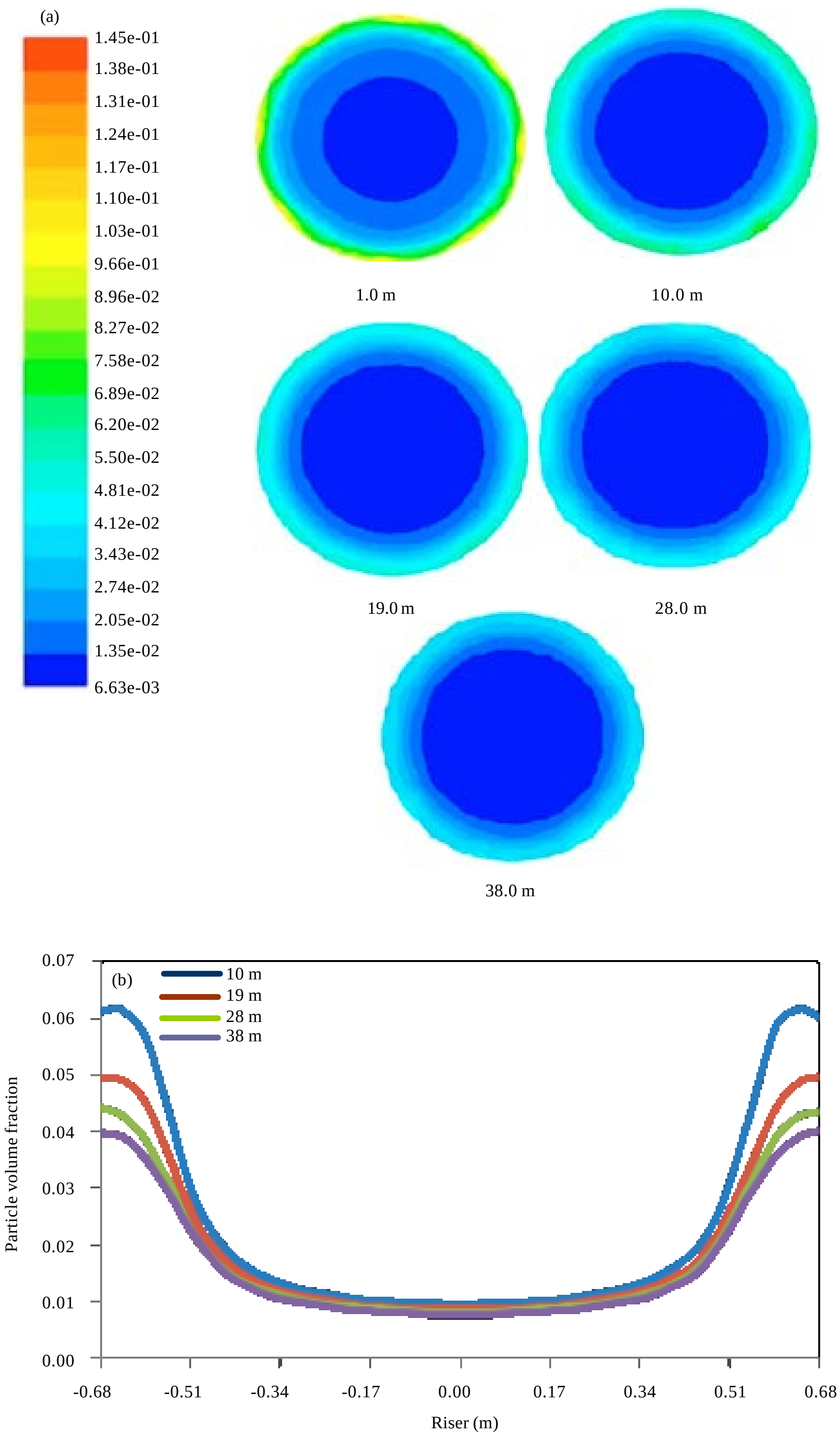

Fig. 3(a-b): Particle volume fraction contours on planes at different levels along the riser (a) Contour and (b) Radial profile

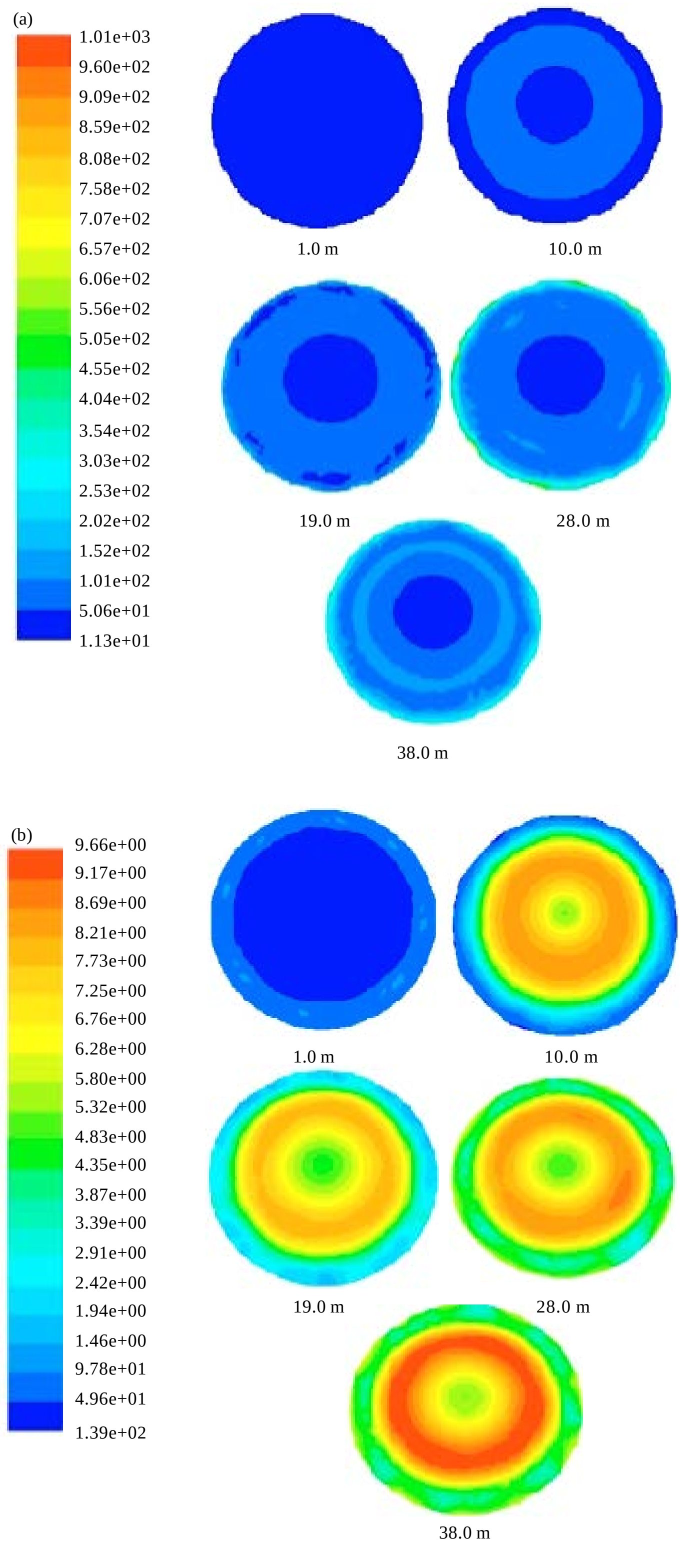

Fig. 4(a-b): Contours of (a) Turbulent dissipation rates and (b) Turbulence kinetic energy of the particle phase

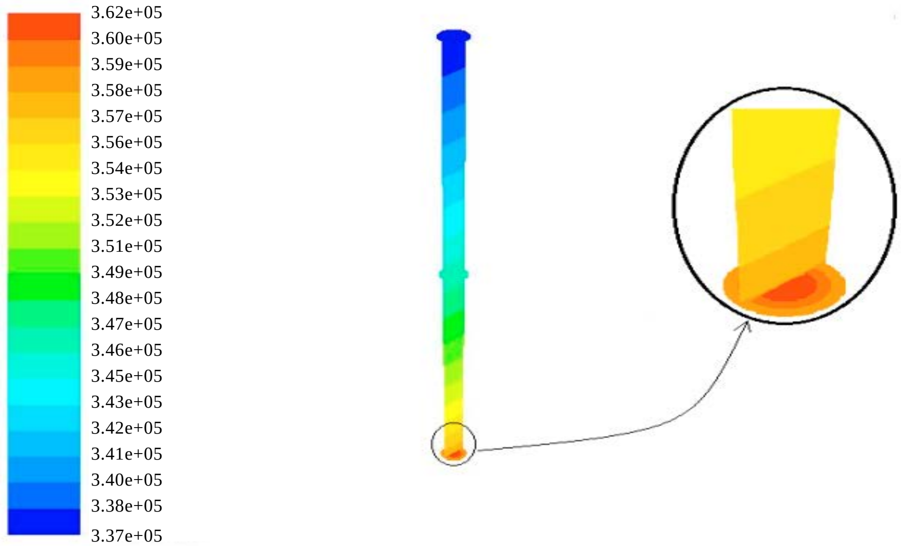

Fig. 5: Absolute pressure of the fluidized bed along the riser

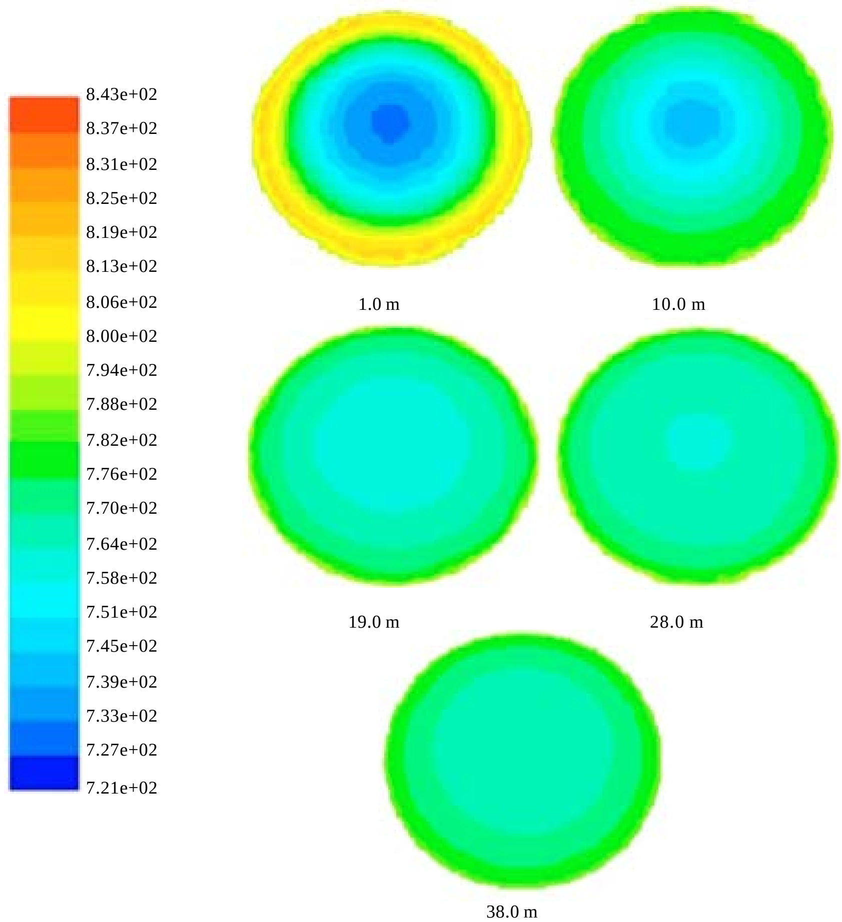

Fig. 6: Temperature distribution of solid phase

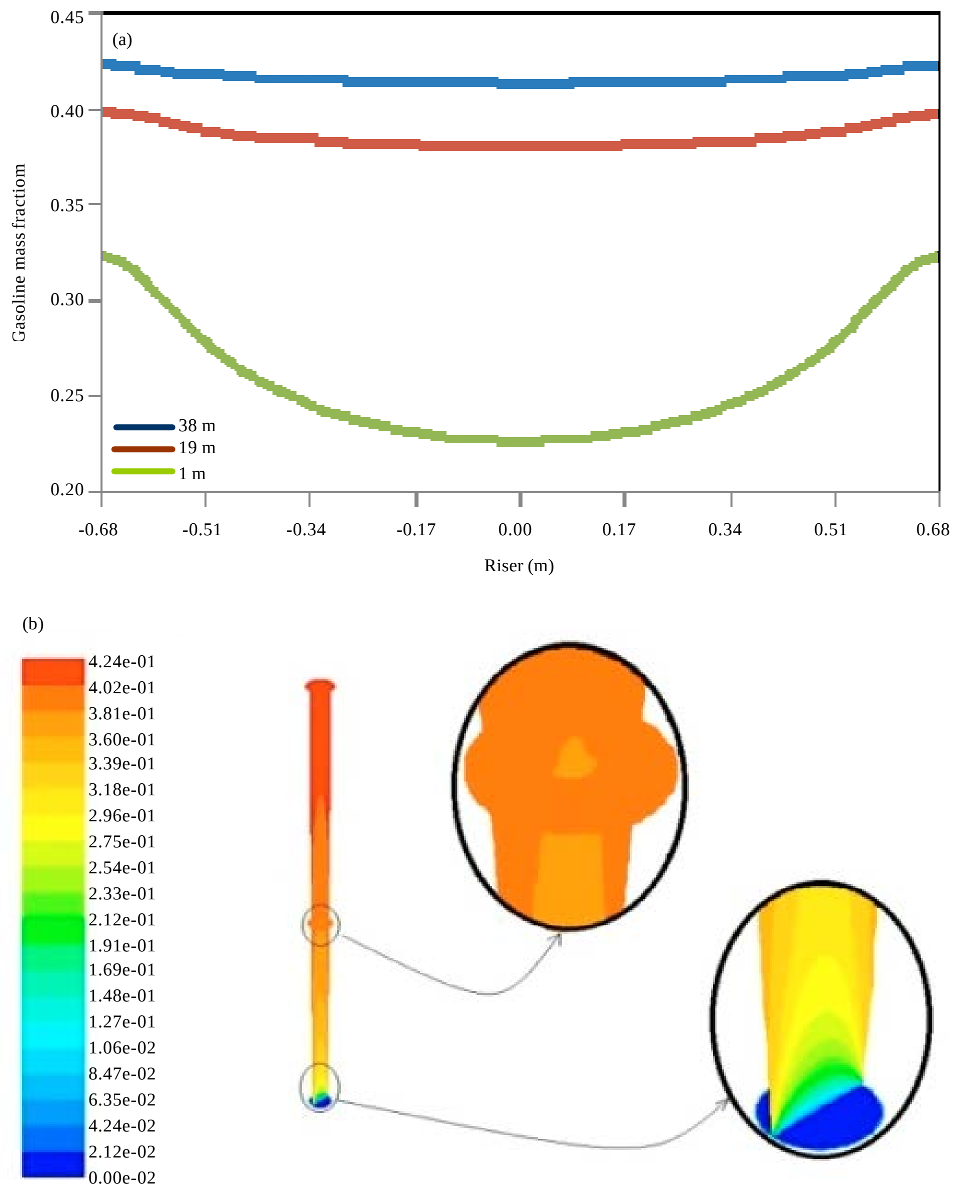

Fig. 7(a-b): Gasoline mass fraction (a) Radial change at diferent levels across the riser length and (b) Contour

near the wall. This is due to the accumulation of catalyst particles with its very high temperature near the wall. Uniform temperature is obtained in the upper half of the riser.

As can be expected, the conversion is higher near the wall than at the center (in the annulus region), especially at the bottom of the riser. This is obvious in Fig. 7a-b where gasoline yield increases radially towards the wall. The concentration of products changed slightly at the upper half of the riser (almost constant) indicating that most of the cracking reactions occur at the feed injection zone showing that the oil cracking is an instantaneous reaction. As it is required to increase the yield of gasoline, LPG and propylene products, it is also required to decrease the yields of the by-products coke and dry gas. Their distribution in the riser is almost same, as shown in Fig. 8.

Table 4 shows that, the average mass fraction of gasoline and coke agrees with the industrial RFCC yield

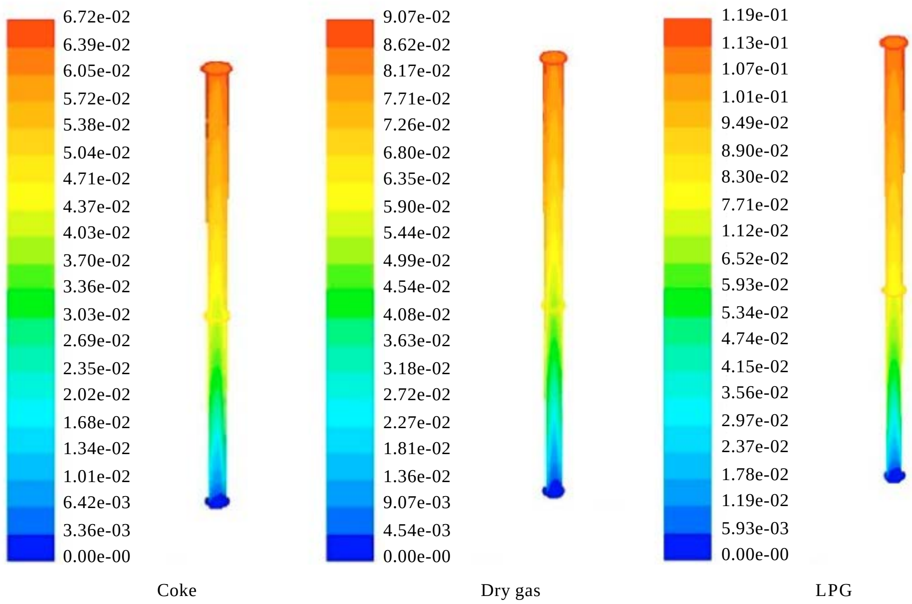

Fig. 8: Contours of coke and dry gas mass fraction

Table 4: Comparison of the outlet average mass fractions between simulated and industrial RFCC unit

Products (species)	Area average mass fraction (3D model)	Industrial plant yield
AR	1.97e-07	
HFO	0.00911	
Slurry (fuel or decant oil)	0.00911	0.0469
Diesel (LFO)	0.28582	0.2152
Gasoline	0.44527	0.4433
LPG	0.12155	0.1544
Dry gas	0.0789	0.0441
Coke	0.05934	0.0932
Losses	0.0	0.0050

while a higher yield of dry gas is obtained. This can be from the flexibility of using same kinetic parameters for different feedstocks.

CONCLUSION

The 3D model incorporating the kinetic theory for solid particles used in FLUENT 14 together with the 7-lump kinetic model is used to simulate the industrial RFCC riser complex hydrodynamics and kinetics. It predicts well the trends and behavior that are observed in the industrial riser for the velocity and temperature profiles. At the oil catalyst contact zone (below 10 m), the riser exhibits high temperature near the wall and lower temperature in the center core due to the fast reactions in this zone. Also the profiles are not uniform as in the rest length of the riser.

ACKNOWLEDGMENT

Authors are grateful to Universiti Teknologi PETRONAS for providing all the support to undertake this research study.

REFERENCES

Almuttahar, A. and F. Taghipour, 2008. Computational fluid dynamics of high density circulating fluidized bed riser: Study of modeling parameters. Powder Technol., 185: 11-23.

Behjat, Y., S. Shahhosseini and M.A. Marvast, 2011. Simulation study of droplet vaporization effects on gas-solid fluidized bed. J. Taiwan Inst. Chem. Eng., 42: 419-427.

Berry, T.A., T.R. McKeen, T.S. Pugsley and A.K. Dalai, 2004. Two-dimensional reaction engineering model of the riser section of a fluid catalytic cracking unit. Ind. Eng. Chem. Res., 43: 5571-5581.

Das, A.K., E. Baudrez, G.B. Marin and G.J. Heynderickx, 2003. Three-dimensional simulation of a fluid catalytic cracking riser reactor. Ind. Eng. Chem. Res., 42: 2602-2617.

ENSPM, 1999. Refining Petrochemicals Chemicals Engineering Data Book. ENSPM Formation Industry, France.

Gidaspow, D., 1994. Multiphase Flow and Fluidization: Continuum and Kinetic Theory Descriptions. Academic Press, Boston, MA., USA.

Gunn, D.J., 1978. Transfer of heat or mass to particles in fixed and fluidised beds. Int. J. Heat Mass Transfer, 21: 467-476.

Hodapp, M.J., J.J. Ramirez-Behainne, M. Mori and L. Goldstein, 2012. Numerical studies of the gas-solid hydrodynamics at high temperature in the riser of a bench-scale circulating fluidized bed. Int. J. Chem. Eng., 10.1155/2012/786982

Huilin, L., D. Gidaspow, J. Bouillard and L. Wentie, 2003. Hydrodynamic simulation of gas-solid flow in a riser using kinetic theory of granular flow. Chem. Eng. J., 95: 1-13.

Lan, X., C. Xu, G. Wang, L. Wu and J. Gao, 2009. CFD modeling of gas-solid flow and cracking reaction in two-stage riser FCC reactors. Chem. Eng. Sci., 64: 3847-3858.

Lopes, G.C., L.M. Rosa, M. Mori, J.R. Nunhez and W.P. Martignoni, 2011. Three-dimensional modeling of fluid catalytic cracking industrial riser flow and reactions. Comput. Chem. Eng., 35: 2159-2168.

Meyers, R.A. and D.A. Hunt, 2003. Handbook of Petroleum Refining Processes. McGraw-Hill, USA.

Pekediz, A., D. Kraemer, A. Blasetti and H. de Lasa, 1997. Heats of catalytic cracking. Determination in a riser simulator reactor. Ind. Eng. Chem. Res., 36: 4516-4522.

Sadeghbeigi, R., 2012. Fluid Catalytic Cracking Handbook: An Expert Guide to the Practical Operation, Design and Optimization of FCC Units. Elsevier, USA., ISBN-13: 9780123869654, Pages: 361.

Shah, M.T., R.P. Utikar, M.O. Tade and V.K. Pareek, 2011. Hydrodynamics of an FCC riser using energy minimization multiscale drag model. Chem. Eng. J., 168: 812-821.

Theologos, K.N., A.I. Lygeros and N.C. Markatos, 1999. Feedstock atomization effects on FCC riser reactors selectivity. Chem. Eng. Sci., 54: 5617-5625.

Xu, O.G., H.Y. Su, S.J. Mu and J. Chu, 2006. 7-lump kinetic model for residual oil catalytic cracking. J. Zhejiang Univ. Sci. A., 7: 1932-1941.

Zheng, Y., X. Wan, Z. Qian, F. Wei and Y. Jin, 2001. Numerical simulation of the gas-particle turbulent flow in riser reactor based on k-ε-k_p-ε_p-θ two-fluid model. Chem. Eng. Sci., 56: 6813-6822.