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Validation of Reacting Flow Model for RFCC Riser in Khartoum Refinery

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Abstract

The flow behavior and catalytic cracking reactions in the riser of an industrial Residue Fluid Catalytic Cracking (RFCC) unit in Khartoum Refinery Company (KRC) Sudan are modeled in a multi–fluid Eulerian model. In this riser atmospheric residue is cracked into diesel, gasoline, lighter gases and coke over zeolite catalyst surface. The CFD model is developed for the solid–gas flow in the riser and solved using ANSYS FLUENT in Workbench 14. For the hydrodynamic model, the $k-\varepsilon$ gas–solid turbulent flow per phase model is used, and the particle–level fluctuations are modeled in the framework of the kinetic theory of granular flow (KTGF) to simulate the flow in the riser. Lump kinetics models are used to describe the residue catalytic cracking reactions. On validating this hydrodynamic model, the particle volume fraction and velocity profiles show very good agreement with the published experimental data. Also the comprehensive model agrees very well with the industrial RFCC plant data

Keywords: ANSYS Fluent; Lump kinetics; Granular Flow; 7-lumps; heat of reaction.

Introduction

Heavy refinery oils are converted into more valuable gasoline and lighter products by catalytic cracking process using zeolite catalyst in fluidized bed. The evolution of Fluid Catalytic Cracking (FCC) process leads to the new developments where heavier feeds like atmospheric residues are processed. Residual oil Fluid Catalytic Cracking (RFCC) units charge the high Conradson carbon residue and metal-contaminated feedstocks, such as atmospheric residues or mixtures of vacuum residue and gas oils to maximize gasoline production [1]. Many researchers have modeled the hydrodynamics and kinetics of gas oil catalytic cracking in FCC units [2, 3, 4, 5]. Very few of them study the RFCC riser model. One of the most important aspects in understanding heavy oil catalytic cracking reactions is the chemical kinetics study. Flow dynamics and chemical kinetics simultaneously describe well the process in the FCC (RFCC) riser. Some researchers employ the CFD modeling for the FCC riser reactors to study the model of two-phase reacting flow without considering turbulence and diffusion of particle phase [6]. Kinetic theory of granular flow was used by other researchers to study the gas-particle turbulent flow and hydrodynamics [7, 8, 9, 10]. They didn't consider the reactions kinetics model. The hydrodynamics and kinetics models are simultaneously studied by Lan *et al*. [11] and Das *et al*. [12] for gas oil FCC unit.

Although modeling tools help to explain the fluid behavior more accurately, experimental studies are required to validate multiphase CFD model. Particle velocities and concentrations are particularly essential to determine different fluidization properties such as suspension densities, local solid flux, and solid effective viscosities. Until 1987, dense flow hydrodynamic experiments measured either the particle velocities or the particle concentrations only [13]. The study by Bader *et al*. [14] appears to be the first in which both the particle velocities and the particle concentrations were determined for the riser flow. Since then, researchers have been able to compare and validate their theoretical models with experimental studies [15]. In general, most of the studies reported on CFD modeling of FCC/RFCC riser lack model validation with laboratory scale experimental and/or industrial plant data.

Riser Model Development:

In the present model, the vaporization of the feed is assumed to be instantaneous, hence the vapour and catalyst inlet temperatures are estimated at the point of contact [4, 16]. The catalyst particles were assumed to be spherical with average diameter and have

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homogeneous distribution inside the dense and dilute phases. Both phases are assumed to be in plug flow conditions. For the gas-solid upward flow system in the riser, the steady-state mass, momentum and energy conservation equations for each phase (governing equations in Table 1) are developed for simultaneous solution using the Eulerian - Eulerian approach in ANSYS Fluent 14. The $k-\varepsilon$ gas–solid turbulent flow per phase model is used to model the riser hydrodynamics, and the particle–level fluctuations are modeled in the framework of the kinetic theory of granular flow (KTGF) to simulate the flow in the riser.

Table 1: The two phase three dimension conservation equations

Gas Phase		
Continuity	$\nabla.\left(\varepsilon_g\rho_g\boldsymbol{v}\right)=0$	(1)
Component Continuity	$\nabla.\ \left(\varepsilon_g\rho_g C_j\boldsymbol{v}\right)=\nabla.\ \left(D_m\varepsilon_g\rho_g\ (\nabla.C_j\ )\right)\ +r_j \qquad (\forall j=1,\dots,14)$	(2)
Momentum	$\nabla.\ \left(\varepsilon_g\rho_g\boldsymbol{v}.\boldsymbol{v}\right)=-\nabla.\ \left(P+\frac{2}{3}\rho_g k\right)-\nabla.\ \left(\varepsilon_g\boldsymbol{\tau}_g\right)+\varepsilon_g\rho_g g-\beta(\boldsymbol{v}-\boldsymbol{V})$ with viscous stresses: $\boldsymbol{\tau}_g=-\left[\left(\xi_g-\frac{2}{3}\mu_g\right)(\nabla.\ \boldsymbol{v})+\left(\mu_g+\mu_g^t\right)[\nabla.\ \boldsymbol{v}+\ (\nabla.\ \boldsymbol{v})^T]\right]$	(3)
Energy	$\nabla.\ \left(\varepsilon_g\rho_g H_g\boldsymbol{v}\right)=\nabla.\ \left[\varepsilon_g(\lambda+\lambda^t)\ \nabla.\ T\right]-\nabla.\ \left(\left(P+\frac{2}{3}\rho_g k\right)\boldsymbol{v}\right)-$ $\nabla.\left(\varepsilon_g\boldsymbol{\tau}_g\ .\ \boldsymbol{v}\right)-\frac{\beta}{2}(\boldsymbol{v}.\boldsymbol{v}-\boldsymbol{V}.\boldsymbol{V})+h_f a_v(T_s-T)+\varepsilon_g\rho_g\boldsymbol{g}\ .\ \boldsymbol{v}-\beta\left(k-\frac{3}{2}\theta\right)$	(4)
Solid Phase		
Continuity	$\nabla.\ \left(\varepsilon_s\rho_{sp}\boldsymbol{V}\right)=0$	(5)
Momentum	$\nabla.\ (\varepsilon_s\rho_s\boldsymbol{V}\ .\ \boldsymbol{V})=-\nabla.\ P_s-\nabla.\ (\varepsilon_s\boldsymbol{\tau}_s)+\varepsilon_s\rho_s g+\beta(\boldsymbol{v}-\boldsymbol{V})$ with solid phase stresses $\boldsymbol{\tau}_s=-\left[\left(\xi_s-\frac{2}{3}\mu_s\right)(\nabla.\ \boldsymbol{V})+\mu_s\left[[\nabla.\ \boldsymbol{V}+\ (\nabla.\ \boldsymbol{V})^T]\right]\right]$	(6)
Granular Temperature	$\frac{3}{2}\ \nabla.(\varepsilon_s\rho_s\theta\boldsymbol{V})=\ -(P_s\boldsymbol{I}+\varepsilon_s\boldsymbol{\tau}_s):\nabla\boldsymbol{V}-\nabla.(\varepsilon_s\boldsymbol{q})-3\beta\theta-\gamma$	(7)
Turbulence	(in both phases, replacing the subscript g with s for solid)	
Turbulent kinetic energy	$\nabla.\left(\varepsilon_g\rho_g k\boldsymbol{v}\right)=\nabla.\ \left[\varepsilon_g(\frac{\mu_g+\mu_g^t}{\sigma_k})\nabla k\right]+\left[\varepsilon_9\mu_g^t[\nabla.\ \boldsymbol{v}+\ (\nabla.\ \boldsymbol{v})^T]\right]:(\nabla.\ \boldsymbol{v})-$ $\varepsilon_g\rho_g\epsilon-2\beta k$	(8)
Turbulence dissipation energy	$\nabla.\left(\varepsilon_g\rho_g\epsilon\boldsymbol{v}\right)=\nabla.\ \left[\varepsilon_g(\frac{\mu_g+\mu_g^t}{\sigma_\epsilon})\nabla\epsilon\right]+C_{1\epsilon}\frac{\epsilon}{k}\left[\varepsilon_9\mu_g^t[\nabla.\ \boldsymbol{v}+\ (\nabla.\ \boldsymbol{v})^T]:(\nabla.\ \boldsymbol{v})\right]-$ $C_{2\epsilon}\varepsilon_g\rho_g\frac{\epsilon^2}{k}-2\beta k$	(9)

A 7-lump kinetic model considering all the products and coke as separate lumps proposed by Xu *et al.*, [17] is chosen in the present work. Lump description, reaction scheme and model equation are detailed in our previous paper [18]. Previously a constant value for an average heat of reaction in kJ per kg coke was used in different studies [11]. In this study, the heats of the 18 reactions were calculated from the standard heats of formation and heats of vaporization of the species that tabulated in Table 2. Ahmed *et al.*, [18] also tabulated the calculated heats of reactions, the operating conditions and the CFD numerical parameters. The hexahedral mesh for the three-dimension model is sized in a grid independent test that resulted in the use of a body size 0.05 with 468160 elements. Also the quadrilateral mesh size (100 × 500) is used in the two dimensional model. The wall Yplus value is better in finer grids.

Table 2: The lumps description and properties

Lump	Boiling range	Average Mw	ΔH_f^o (kJ/kmol)	ΔH_f (kJ/kmol)	ΔH_{vap} (kJ/kg)	C_P *10^{-3} (kJ/kg K) [b]
Residue (AR)	≥500 °C	950	- 938348 [a]		238 [a] (extrapolation)	$-180.6 + 6.38\,T - 0.002\,T^2$
Heavy Fuel Oil (HFO)	350 - 500 °C	386	- 669602.5 [a]		248 [a]	$-615.8 + 8.746\,T - 0.007\,T^2$
Light Fuel Oil (LFO)	220 - 350 °C	229	- 358577 [a]		258 [a]	$-841.2 + 9.495\,T - 0.008\,T^2 + 1.26e^{-6} T^3$
Gasoline (GO)	C5 - 200 °C	117.8		- 134741.2 [b]		$-895.7 + 10.8\,T - 0.011\,T^2 + 5e^{-6}\,T^3$
Liquefied Petroleum Gas (LPG)	C3 + C4	46.7		- 9332.995 [b]		$-84.26 + 7.739\,T - 3.82e^{-8}\,T^2 + 7.29e^{-11} T^3$
Dry gas (DG)	C1 + C2 + H_2 + H_2S	18.4		+ 18876.192 [b]		$413.17 + 3.526\,T - 1.245e^{-3}\,T^2 + 1.26e^{-11} T^3$
Coke		400	2425 (of graphite)	+ 247376		

a= From Pekediz et al [19]
b= From Data Book [20]

Hence the above model for the fast fluidization flow in the industrial RFCC riser determines the degree of interphase coupling for gas and particles through KTGF models. It also can describe the particles turbulence as well as the gas turbulence. The 7-lump [17] and 14-lump [11] models are used to define the cracking reactions taking place in the riser. Eulerian-Eulerian approach of FLUENT software is used to solve the 2D and 3D models and simulate the industrial RFCC riser. The 2D and 3D geometries are meshed in the pre-processor software of ANSYS workbench 14. The pressure based FLUENT solver is used to solve the governing and constitutive equations of the comprehensive model using Phase Coupled SIMPLE (PCSIMPLE) algorithm. The hydrodynamic model is solved simultaneously with the kinetic model in species transport 2D axisymmetric and 3D models. The KTGF models are used to simulate the fast fluidization regime in the riser. Species properties are accurately estimated and solution parameters are carefully defined to the cases to ensure the accuracy and fast convergence in solving the model.

Model Validation with Experimental Data

In the past decades, a great deal of experimental work has discovered some important flow phenomena in risers such as the irregular radial distributions of particles, back flow of the particles near the wall and segregations of particles. It is important to explain these flow behaviors for the industrial application of the risers [8]. Therefore, the turbulent flow model of this work is validated with the experimental data of Bader *et al*. [14], Yang [21] and Zheng *et al*. [8].Table 3 shows the operating conditions and riser dimensions for all the above works. Lan *et al*. [11] validate their model with both Bader *et al*. [14] and Yang [21], therefore comparison with their validation results is shown.

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Table 3: Operating conditions used for comparison

Operating conditions	**Yang (1991)**	**Bader *et al.* (1988)**	**Zheng *et al.* (2001)**
Catalyst type	FCC	Grace US-260	N/A
Particle diameter (μm)	54	76	77
Particle density (kg/m^3)	1545	1714	1398
Particle mass flux(kg/m^2 s)	92	98	33.4
Superficial gas velocity, m/s	4.33	3.7	4.33
Riser inside diameter, m	0.14	0.305	0.418
Riser hight, m	11	11.505	18

The model shows good agreement with the experimental data in the solid phase velocity and volume fraction comparison, as illustrated in Figures 1, 2 and 3. Zheng *et al*. [8] adopted three models, A: k-ε-k_p-ε_p-Θ model. B: k-ε- Θ model. C: k-ε-k_p-ε_p-Θ model in which the dissipation of the turbulent energy transferred between gas and solid phases was neglected. Therefore comparison with their two models A and C are shown in Figure 3. A smaller specularity coefficient generally denotes a smooth wall with less friction, therefore values of this coefficient strongly affect the gas back-mixing for bubbling and slugging fluidized beds [22]. For circulating fluidized beds of the chosen experimental works with flow regimes between turbulent and fast fluidization, the core annulus flow with near wall back-mixing is hardly predicted with the reported values of specularity and particle wall restitution coefficient. Figure 2 shows that the predicted particle velocity profile and volume fraction that results from the 3D model represent Bader *et al*. [14] experimental data better than that predicted from the 2D model. While both models predict better profiles representing Yang [21] experimental data than the 2D model of Lan *et al*. [11] as shown in Figure 1.

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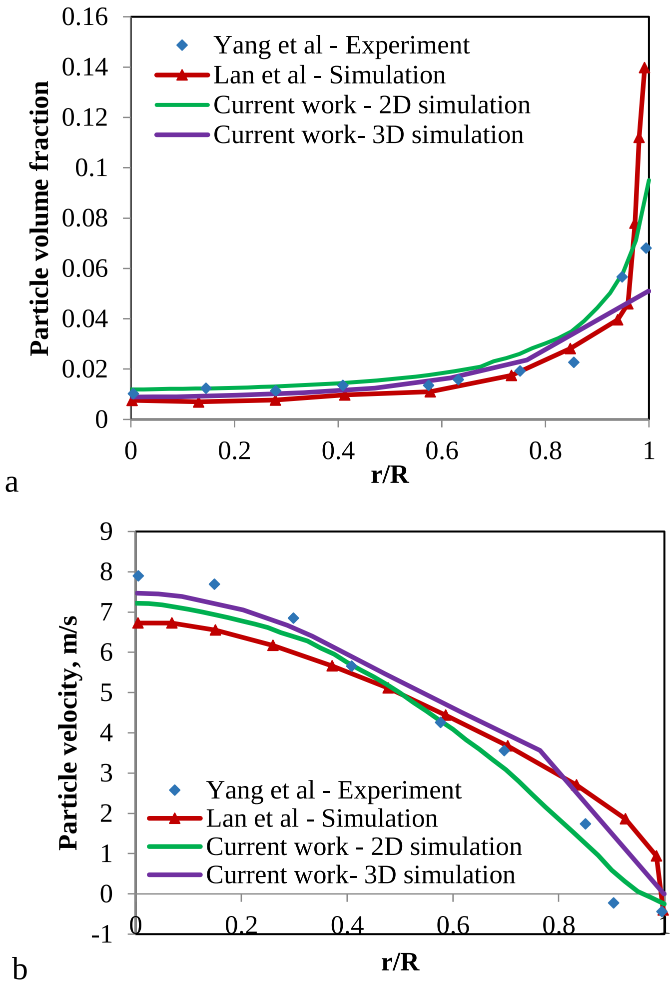

Figure 1: Comparison of particle volume fraction (a) and particle velocity (b) at the 5.6 m riser level between the predicted models and the experimental data of Yang [21]

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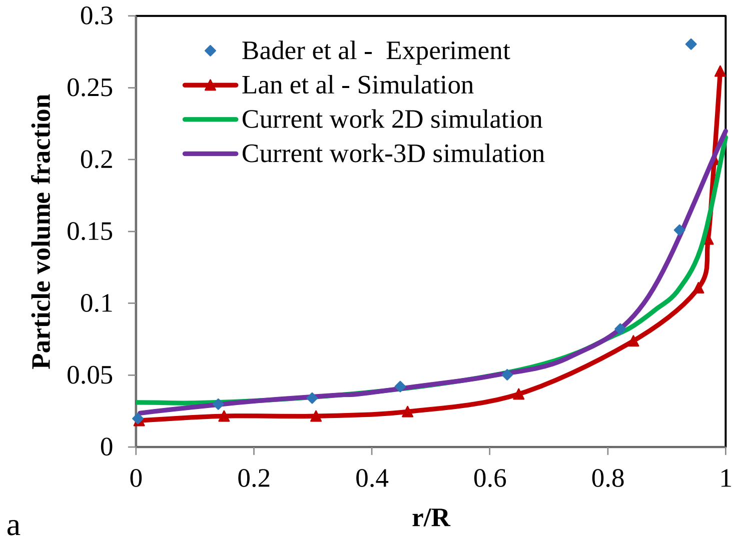

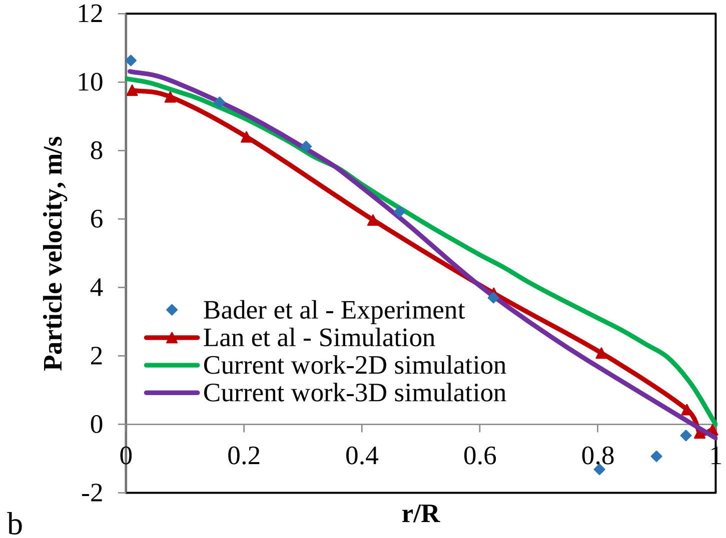

Figure 2: Comparison of particle volume fraction (a) and particle velocity (b) at the 4 m riser level between the predicted models and the experimental data of Bader *et al*. [14]

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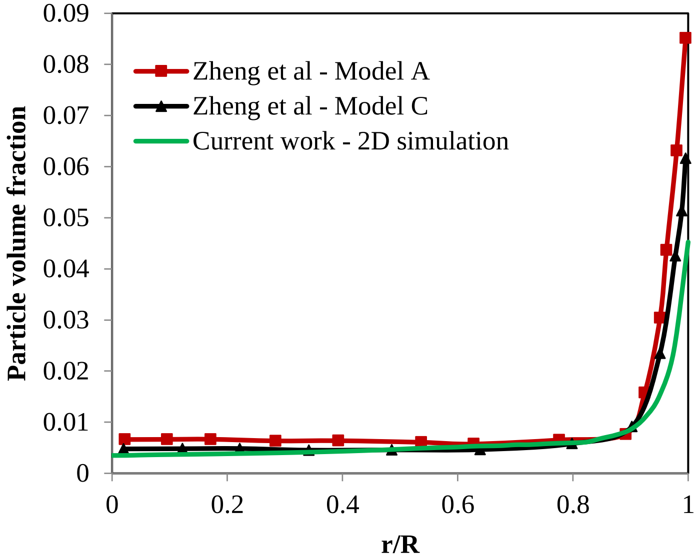
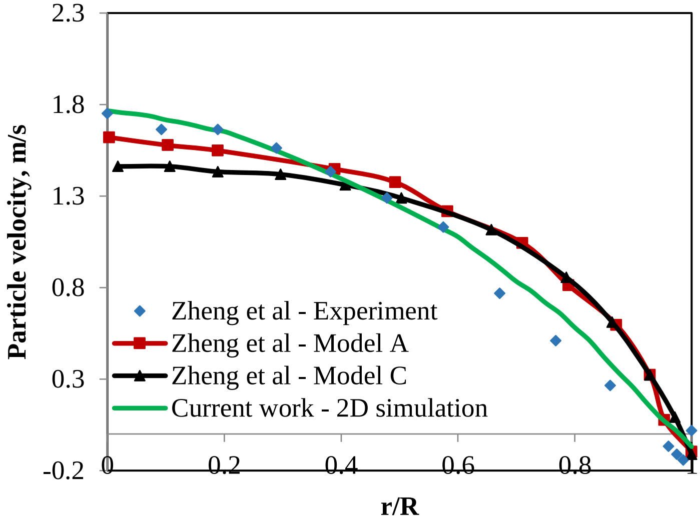


a



b

Figure 3: Comparison of particle volume fraction (a) and particle velocity (b) at the 14.05 m riser level between the predicted model and the experimental data of Zheng et al. [8]

Validation of the reacting flow total model (*i.e* both hydrodynamic and kinetic models) is lacking in the literature. Therefore comparison with the simulation work of Lan *et al*. [11] is described. Table 4 shows the operating conditions and riser dimensions of their work and of the industrial plant.

Table 4: Operating conditions for comparison with Lan *et al*. [11] works

Operating conditions	**Lan et al. 1st stage riser**	**Industrial RFCC riser**
Catalyst type	Zeolite	Zeolite
Particle diameter (μm)	76	76
Particle density (kg/m^3)	1714	1700
Particle mass flux(kg/m^2 s)	230	320
Superficial gas velocity, m/s	4.7	5.75
Riser inside diameter, m	0.35	1.36
Riser hight, m	12.81	38
Reaction temperature, ºC	500	508
Reaction pressure, kPa	299.55	361.3
COR	5.46	6.88
Pre-lift steam, kg/s	0.12	2.46

The simulation results from modeling the riser of Lan *et al*. [11] are shown in Figure 4. The flow behavior at the wall has been found to be slightly different from their published results which may be attributed to the differences in gas properties of the 14 lumps used. In our previous papers [18, 23] more accurate species properties were found from data books and Aspen HYSYS 7.3 data base. Although the simulation results in Figure 4 are not consistent with the results of Lan *et al*. [11], it resembles the trend of the particle volume fraction and velocity profiles of the experimental results of both Bader *et al*.[14] and Yang [21] representing the annular - core flow structure in the riser.

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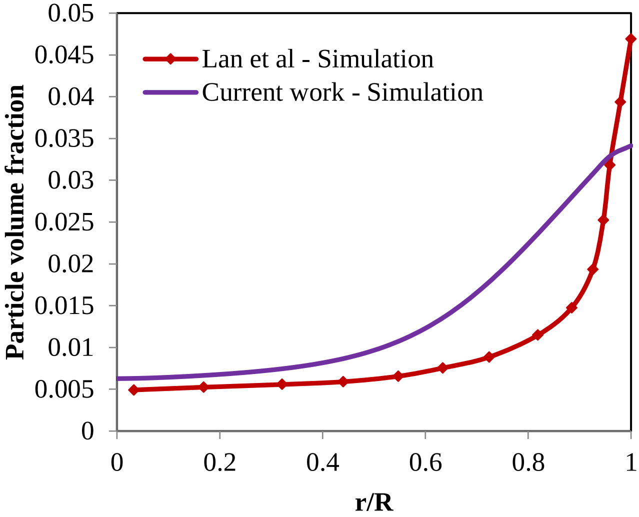
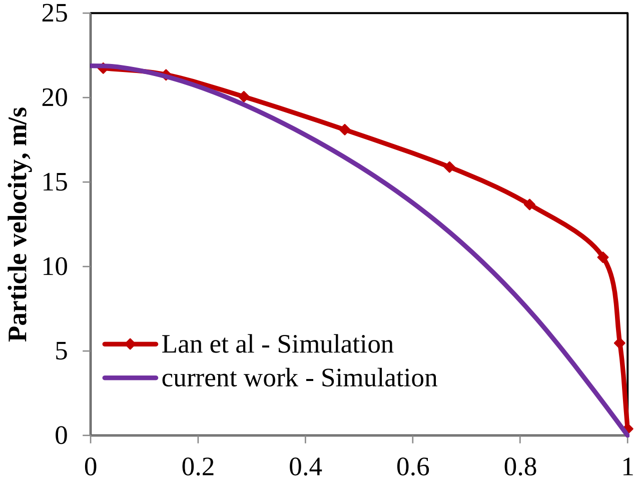


a



b

Figure 4: Comparison of particle volume fraction (a) and particle velocity (b) at the riser outlet between the predicted model and simulation results of Lan *et al*. [11]

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Model Validation with Industrial Plant Data

The predicted axial static temperature profiles of the solid phase along the riser length from simulation cases are compared in Figure 5. For the 2D model cases, better results are found that agree with the industrial RFCC riser fluidized bed temperature in the upper two third length of the riser with the calculated heats of reaction than with the reported heat of reaction. Much better results are obtained on extending the simulation to 3D modelling. It can be observed from Figure 5 that the resulted temperature profile from the 3D model matches the changes in the industrial riser bed temperature along the whole riser especially in the contact zone. The sharp decrease in the solid temperature at the inlet is due to the assumption of instantaneous vaporization. At the contact zone the temperature decreases more since it represents the temperature at the centre core where dilute phase appears suddenly. Almost all the catalyst is driven upward and towards the wall with its high temperature by the explosion of gases. After 3-7 meters the dilute phase of the centre core mixes with the dense phase of the wall, bringing the temperature to a little bit higher than at the contact zone.

Also the average mass fraction of the species at the riser outlet from the 2D and 3D models is compared with the products yield of RFCC unit as obtained from KRC. Table 5 shows that, better results are found with the 3D model. In the industrial RFCC units the yield of gasoline, coke and dry gas are very important. It is required to maximize gasoline yield and minimize both coke and dry gas production in spite of the severe operating temperature and the high feed content of carbon residue. Comparison results in negligible errors for gasoline, coke and dry gas yield. Table 5 validates the 3D, 7-lump model which can be used in simulation and optimization.

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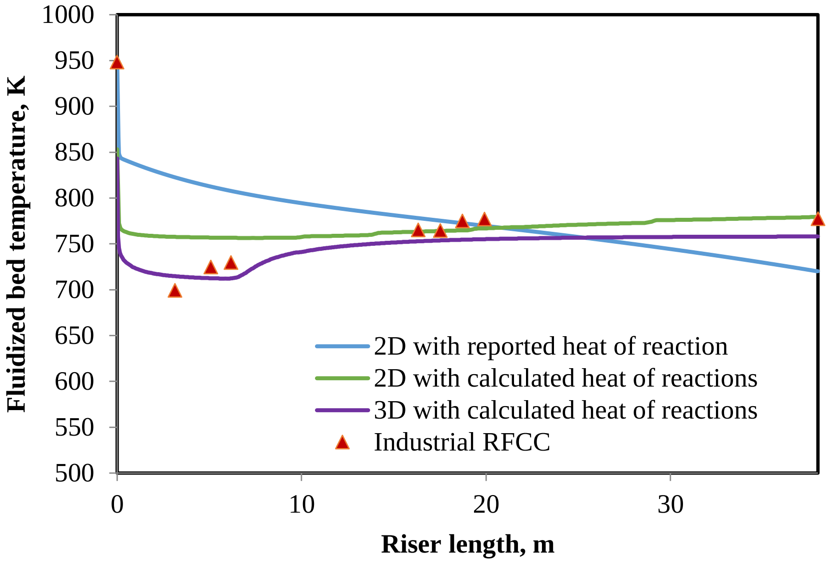

Figure 5: Comparison of solid phase static temperature profile resulted from simulation cases of 2D and 3D models when using reported and calculated heat of reactions

Table 5: Comparison of the outlet average mass fraction between 2D and 3D models (7-lump) and the industrial RFCC unit

Products (species)	**Area average mass fraction(2D model)**	**Area average mass fraction (3D model)**	**Industrial plant yield**
AR	8.76e-08	6.547e-08	
HFO	0.00589	0.00549	
Slurry (Fuel or decant oil)	0.00589	0.00549	0.0469
Diesel (LFO)	0.25328	0.2882	0.2152
Gasoline	0.4355	0.4425	0.4433
LPG	0.143	0.12445	0.1544
Dry Gas	0.0785	0.04039	0.0441
Coke	0.0835	0.09901	0.0932
Losses	0.0	0.0	0.005

Conclusion

The model is validated with published experimental data and its results are also compared with a reported 2D simulation results. The good agreement with the experimental data is observed. Also based on the comparison of concentration and temperature profiles with industrial plant data, the 3D simulation model has been found to be describing the industrial RFCC riser better. Therefore the 3D model can be used validly to optimize some of its process variables.

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