Numerical Simulation and Optimization of an Industrial Fluid Catalytic Cracking Regenerator

Guangwu Tang

Center for Innovation through Visualization and
Simulation,
Purdue University Northwest
2200 169th Street
Hammond, IN, 46323
219-671-3423 Email: tangg@pnw.edu

Bin Wu

Center for Innovation through Visualization and
Simulation,
Purdue University Northwest
2200 169th Street
Hammond, IN, 46323
219-989-3157 Email: wu7@pnw.edu

Dwight Agnello-Dean

BP Company North America
East Chicago, IN 46323
219-787-3446 Email: Dwight.Agnello-Dean@bp.com

Qingjun Meng

BP Refining and Logistics Technology
Naperville, IL, 60563
219-787-3446 Email: qingjun.meng@bp.com

Chenn Q. Zhou (Corresponding Author)

Center for Innovation through Visualization and
Simulation,
Purdue University Northwest
2200 169th Street
Hammond, IN, 46323
219-256-2665 Email: czhou@pnw.edu

Armin K. Silaen

Center for Innovation through Visualization and
Simulation,
Purdue University Northwest
2200 169th Street
Hammond, IN, 46323
219-989-3157 Email: asilaen@pnw.edu

Dong Fu

Center for Innovation through Visualization and
Simulation,
Purdue University Northwest
2200 169th Street
Hammond, IN, 46323
219-989-3157 Email: fudong1985@gmail.com

Joseph Wilson

BP Refining and Logistics Technology
Naperville, IL, 60563
219-787-3446 Email: Joseph.Wilson2@bp.com

Samir Khanna

BP Refining and Logistics Technology
Naperville, IL, 60563
219-787-3446 Email: samir.khanna@bp.com

Abstract: Fluid catalytic cracking (FCC) is one of the most important conversion processes in petroleum refineries. FCC regenerator is a key part of an FCC unit to recover the solid catalyst reactivity by burning off the deposited coke on the catalyst. In this paper, a three-dimensional multi-phase, multi-species reacting flow computational fluid dynamics (CFD) model was established to simulate the flow and the reactions inside an FCC regenerator. The Euler-Euler approach, where the two phases (gas and solid) are considered to be continuous and fully interpenetrating, is employed. A modified drag force model was applied on the CFD model with appropriate influential cluster diameters of particle grouping phenomenon. The developed CFD model was validated by using plant data. With the validated CFD model, the flow characteristics and the inner-phase and inter-phase reactions were studied. The results showed that the effect of oxygen enrichment on the catalysts recovery efficiency was limited when the oxygen enrichment exceeded 5%.

Key Words: Regenerator, CFD, Eulerian, Kinetic theory, Drag model, Hydrodynamics, Combustion.

1 Introduction

Fluid Catalytic Cracking (FCC) process is one of the most important processes in petroleum refinery, which has paid considerable attention over the past 70 years [1]. FCC units play a pivotal role in petroleum refining industry that mainly converts low-value, high-boiling feedstock like gas oil into valuable products such as gasoline and middle distillates by using cracking catalyst [2,3]. The FCC zeolite catalyst particles belong to Group A particles which have mean size and density ranges of $d < 500\mu\text{m}$, $1.4 \text{ g/cm}^3 < \rho < 4 \text{ g/cm}^3$, respectively [4]. During the FCC process, the FCC catalyst loses its reactivity due to the deposition of coke which is generated during the complicated chemical reactions. Since there are 40 to 50 tons of solid catalyst circulated in one FCC unit every minute [5], recycling the deactivated catalyst is critical for the entire process to reduce costs. Recovery of the catalyst reactivity by burning off the coke on the catalyst in the FCC regenerator is also important to maintain its cracking efficiency. Therefore, it is of great importance to understand the fluidized-bed flow properties and reactions inside the FCC regenerator to achieve high efficiency and low cost.

Fluidized bed technique is widely used in industrial processes, which has been comprehensively studied and optimized using numerical modeling. Both Lagrangian and Eulerian algorithms are used to simulate the gas-solid two phase flow, which consider the gas phase as a continuum [6-8]. However, Lagrangian algorithm solves the Newtonian equations of motion for each particle and takes into consideration of particle collisions effects. Particle collision laws are applied for the solid-solid collision based on the energy dissipation by means of restitution coefficient and friction [9, 10]. Fluidization phenomena simulation by using Lagrangian algorithm has been reported in lab scale [11]. It is difficult to use Discrete Phase Model (DPM) to model industrial powder process [12]. Lagrangian model also requires more computational resources compared to an Eulerian model and most of the application are limited to big particles ($d > 500\mu\text{m}$) [9,10,13]. Gas and particles are all considered as continuums and fully interpenetrating in Eulerian algorithm. The interactions between two continuous phases are described by generalized Navier-Stokes equations with additional closure laws to describe particle-particle and particle-wall interactions. Kinetic theory of granular flow provides explicit closures for Geldart A particles, such as FCC catalyst, with both efficiency and accuracy [14-19].

The main task for FCC regenerator is to consume the coke (including carbon and hydrogen) on the catalyst surface through combustion and also to elevate the catalyst bulk temperature to ensure optimal conditions for cracking reactions. However, majority of the CFD studies of fluidized bed devices available in the literatures focused on isothermal process [20]. Due to the computational cost, the application of the fundamentals-oriented models, such as the Eulerian-Eulerian multiphase models applying the kinetic theory of granular flow, for simulation of industrial-scale circulating fluidized bed furnaces has been small. [21] Improvements in numerical techniques and computing power have provided opportunities to advance CFD application on simulating the reactions in a fluidized bed. Lu et al. [22-24] studied the heat transfer and hydrodynamics in a fluidized bed using kinetic theory of granular flow without considering reactions. Due to the complexity of multiphase combustion process in fluidized bed which involves homogeneous and heterogeneous reaction process, only few literatures [25-27] considered CFD for combustion in fluidized bed while overlooking three dimensional effects. Adamczyk et al. [28-29] applied a dense discrete phase model to simulation circulating fluidized bed using ANSYS Fluent. For FCC process, only experiments, empirical and semi-empirical 1D and 2D models are reported in studying the reactions in FCC regenerator [30-34]. Therefore, applying the advanced CFD technique on the FCC catalyst regeneration process to optimize the design and operation is of great significance. And the CFD method is expected to substitute empirical models in future [20].

This paper employs Computational Fluid Dynamics (CFD) to simulate a commercial regenerator. Based on the multiphase Eulerian model with kinetic theory of granular flow, the air-catalyst two phase multi-species reacting flow inside the regenerator was modeled. The flow hydrodynamics was also obtained by using a modified drag model to calculate the gas-solid interaction drag force. Restitution coefficient 0.9 was applied to define the solid-solid collision forces [35]. A reaction model which includes homogeneous and heterogeneous combustion was developed to simulate the multiphase reactions, temperature and species distributions in the FCC regenerator. The simulation results are compared with the plant data. The effect of the important parameter, such as oxygen enrichment, on the flow and reactions has been investigated.

2 CFD Model and Methodology

The Euler-Euler approach, in which the two phases (gas and solid) are considered to be continuous and fully inter-penetrating, is employed. The kinetic theory of granular flow was applied in this simulation, with a Reynolds number of approximately 4×10^5 . Gao et al. [18,19] reported that the laminar viscous model was able to accurately predict flows in the same range of Reynolds number. Therefore, the laminar viscous model was applied in this study. Almuttahir et al. [36] also reported that even in the case of high density circulating fluidized bed, laminar model can give better prediction to the hydrodynamics compared to turbulence models. Chang, et al. [37] applied laminar model to calculate viscous force on an industrial turbulent fluidized bed reactor and validated the axial bed density profile with industrial data. Reaction and heat transfer models are needed in order to model the main function of FCC regenerator to recover catalyst cracking reactivity by burning off the coke on the catalysts. Finite-rate model was used for simulating the combustion. Heterogeneous reaction model with Gunn model [38] for interphase heat transfer were incorporated into the model. Finite-rate model combustion model was used for simulating chemical reactions. Both gas phase reaction and gas-solid interface reactions were defined. P1 radiation model was used for modeling the radiation heat transfer. The main reactions considered in this model were carbon oxidization, hydrogen combustion and CO combustion. The reaction rates were included into the model through User Defined Function (UDF) scripts based on the kinetics referred from literatures.

2.1 Governing equations

2.1.1 Conservation of Mass

Gas-phase continuity equation

$$\partial(\alpha_g \rho_g) / \partial t + \alpha_g \rho_g v_g = m_{pg} - m_{gp} + S_g \quad (1)$$

Solid-phase continuity equation

$$\partial(\alpha_p \rho_p) / \partial t + \alpha_p \rho_p v_p = m_{gp} - m_{pg} + S_p \quad (2)$$

where the first term is the time rate of change of gas phase or solid phase, the second term is the advection of the gas phase or solid phase. Each computational cell is shared by gas and solid phase with the total of solid and gas volume fraction is 1.

$$\alpha_p + \alpha_g = 1 \quad (3)$$

2.1.2 Conservation of Momentum

Gas-phase momentum equation

$$\partial \partial t \alpha g \rho g v g + \partial \partial x j \alpha g \rho g v g v g = -\alpha g p + \tau g + \beta u g - u p + \rho g \alpha g g \quad (4)$$

Solid-phase momentum equation

$$\partial \partial t \alpha p \rho p v p + \partial \partial x j \alpha p \rho p v p v p = -\alpha p p + \tau p - \beta u g - u p + \rho p \alpha p g \quad (5)$$

where the terms on the left hand of the equation are the time rate of change of gas or solid phase and advection term. On the right hand of the equation, body force (gravity, pressure), shear force term and phase interaction terms are considered. β is the gas-solid interphase drag coefficient.

The fluctuations that occur in the solid phase are modeled from the kinetic theory of gases modified to account for inelastic collisions between particles.

Solid-phase turbulent fluctuating energy equation

$$32 \partial \alpha p \rho p \Theta \partial t + \nabla (\alpha p \rho p v p \Theta) = -p p I + \tau p : \nabla v p + \nabla \cdot k \Theta \nabla \Theta - \gamma \Theta + \varnothing g p \quad (6)$$

Where $-p p I + \tau p : \nabla v p$ is the generation of energy by the solid stress tensor, $k \Theta \nabla \Theta$ is the diffusion energy, $\gamma \Theta$ the collisional dissipation of energy, $\varnothing g p$ the energy exchange between the gas phase and the particle phase.

In order to close the governing relations, constitutive equations (7) to (17) are used in this model.

Gas-phase stress tensor

$$\tau g = \alpha g \mu g \nabla u g + \nabla u g T + \alpha g (\lambda g - 23 \mu g) \nabla u g I \quad (7)$$

Solid-phase stress tensor

$$\tau p = \alpha p \mu p \nabla u p + \nabla u p T + \alpha p (\lambda p - 23 \mu p) \nabla u p I \quad (8)$$

Solid-phase pressure

$$p p = \alpha p \rho p 1 + 2(1 + e) \alpha p g 0 \Theta \quad (9)$$

Radial distribution function

$$g 0 = 1 - \alpha p \alpha p, \max 13 - 1 \quad (10)$$

Granular temperature

$$\Theta = 13 u p ' u p ' \quad (11)$$

Solids phase shear viscosity (Gidaspow kinetic theory)

$$\mu_p = 10 \rho_p d_p \pi \Theta^{96} (1+e)^g \Theta^{01+45(1+e)^g} \alpha_p^2 + 45 \alpha_p^2 \rho_p d_p g \Theta^{0(1+e)\Theta\pi} \quad (12)$$

Solids phase shear viscosity (Syamlal-O'Brien kinetic theory)

$$\mu_p = \alpha_p \rho_p d_p \pi \Theta^6 (3-e)^{1+25(1+e)(3e-1)^g} \alpha_p^2 + 45 \alpha_p^2 \rho_p d_p g \Theta^{0(1+e)\Theta\pi} \quad (13)$$

Solids bulk viscosity

$$\lambda_p = 43 \alpha_p \rho_p d_p g \Theta^{0(1+e)\Theta\pi} \quad (14)$$

Diffusion coefficient (Gidaspow kinetic theory)

$$\Gamma \Theta = 150 \rho_p d_p \pi \Theta^{384} (1+e)^g \Theta^{01+65(1+e)^g} \alpha_p^2 + 2 \alpha_p^2 \rho_p d_p g \Theta^{0(1+e)\Theta\pi} \quad (15)$$

Diffusion coefficient (Syamlal-O'Brien kinetic theory)

$$\Gamma \Theta = 15 \alpha_p \rho_p d_p \pi \Theta^4 (41-3321+e)^{1+351+e} 22e-1 g \alpha_p + 815 \pi (41-3321+e)^{(1+e)\alpha_p g} \quad (16)$$

Collisional dissipation of energy fluctuation

$$\gamma \Theta = 12 (1-e^2)^g \Theta d_p \pi \rho_p \alpha_p^2 \Theta^{3/2} \quad (17)$$

The transfer of the kinetic energy of random fluctuations in the particle velocity from the solid phase to the gas phase is:

$$\phi_{gp} = -3 K_{pg} \Theta \quad (18)$$

A modified drag model was used with considering the clustering phenomenon in both dense dilute phase and dilute phase. The influential cluster diameters in the dense phase and the dilute phase were determined in previous research [39]. The modified drag model is listed in Table 1.

2.1.3 Conservation of Energy

Gas-phase energy equation

$$\partial \alpha_g \rho_g h_g + \nabla \cdot \alpha_g \rho_g h_g \mathbf{u}_g = \alpha_g \partial P_g / \partial t + \tau_g : \nabla \mathbf{u}_g - \nabla q_g + S_g + q = 1/2 (Q_{qg} + m_{qgh} q_g - m_{qgh} q_g) \quad (19)$$

Solid-phase energy equation

$$\partial \alpha_p \rho_p h_p + \nabla \cdot \alpha_p \rho_p h_p \mathbf{u}_p = \alpha_p \partial P_p / \partial t + \tau_p : \nabla \mathbf{u}_p - \nabla q_p + S_p + q = 1/2 (Q_{qp} + m_{qph} q_p - m_{qph} q_p) \quad (20)$$

where ρ_g represents gas phase, ρ_s represents solid phase, ρ_l represent liquid phase, ρ_{any} represents any other two phases except the calculated phase in each equation. h_g is the specific enthalpy of the gas phase, q is the heat flux, S is a source term that includes sources of enthalpy (such as radiation), h_{ex} is the intensity of heat exchange between gas and solid or liquid phase. h_{int} is the interphase enthalpy.

$$Q_{qg} = C_{qg} (T_q - T_g) \quad (21)$$

C_{qg} is the volumetric heat transfer coefficient between solid or liquid phase and gas phase, which related to the phase q Nusselt number, Nu_q .

$$C_{qg} = 6K_g a_{qg} Nu_{qg} d_{qg}^2 \quad (22)$$

K_g is the thermal conductivity of gas phase.

For Gunn heat transfer model [38], the

$$Nu_p = 7 - 10a_g + 5a_g^2 + 0.7Re_p^{0.2}Pr^{1/3} + (1.33 - 2.4a_g + 1.2a_g^2) Re_p^{0.7}Pr^{1/3} \quad (23)$$

$$Pr = c_{pg} \mu_g K_g \quad (24)$$

P1 Radiation Model

In FCC regenerator, another heat transfer form is radiation due to the combustion occurs inside with high temperature around 1000K. Therefore, thermal radiation should be considered. The radiation heat flux as function of incident radiation intensity in P1 model is:

$$q_r = -\frac{1}{3}(a + \sigma_s) - C\sigma_s \nabla G \quad (25)$$

where a is the absorption coefficient, σ_s is the scattering coefficient, G is the incident radiation, C is the linear-anisotropic phase function coefficient.

$$-\nabla q_r = aG - 4a n^2 \sigma T^4 \quad (26)$$

The expression for $-\nabla q_r$ can be directly substitute into the energy equation to account for the heat sources due to the radiation.

2.1.4 Conservation of Species

Species transport equations are used to model the species which are involved in the chemical reactions. For each phase k , predict the local mass fraction of each species, Y_{ik} , through the solution of a convection-diffusion equation for i species, when applied to multiphase mixture can be expressed in the following form:

$$\frac{\partial}{\partial t}(\rho_g Y_{ig}) + \nabla \cdot (\rho_g Y_{ig} \mathbf{u}_g) = -\nabla \cdot (\rho_g \mathbf{u}_g Y_{ig}) + \rho_g (S_{ig} + R_{ig}) + p = 1n(m_{pigi} - m_{gipi}) + Rate \quad (27)$$

where R_{ig} is the net rate of production of homogeneous species i by chemical reaction for gas phase. m_{pigi} is the mass transfer source between species i and j from solid phase to gas phase. $Rate$ is the heterogeneous reaction rate. ρ_g is the volume fraction for gas phase. S_{ig} is the rate of creation by addition from the dispersed phase plus any user-defined sources.

In FCC regenerator, deposited coke on the solid catalyst surface reacts with gas phase species O_2 and CO_2 . Such interphase chemical reactions are also known as heterogeneous reactions. The heterogeneous phase interaction reaction rates used for the reactions [43] are:

$$Rate = k_i = 1NR Y_{ip} VOF_{ip} MW_i \cdot 1000 st \cdot 10^{-3} \text{ kmol m}^{-3} \text{ s}^{-1} \quad (28)$$

$$k = A(T_{ip} T_{ref})^b \exp(-E/R T_{ip}) \quad (29)$$

where, Y_i is i^{th} species mass fraction. NR is the total number of reactants in a given inter-phase reaction. ip is the bulk density of phase ip . VOF_{ip} is the volume fraction of phase ip . MW_i is the molecular weight of the reactant species. st is the stoichiometric coefficient of reactant in the given reaction. k is the rate constant. T_{ip} is phase temperature. T_{ref} is reference temperature. A is pre-exponential factor, and E is activation energy.

2.2 Simulation code and solution method

This simulation was using the commercial software package ANSYS Fluent[®]. The Finite Volume Method (FVM) [44] was used to solve the partial differential equations by discretized the equations using an upwind differencing scheme. The Phase Coupled SIMPLE algorithm was applied to adjust the pressure and velocities after each iteration. The transient approach was used to solve this problem due to the real flow characteristics. UDF scripts were coupled into the main

solver to calculate the flow and reactions. The drag coefficient between the gas phase and solid phase based on previous developed modified drag model was applied by using UDF scripts. The reaction rates for four reactions are based on the heterogeneous reaction rate, which were also written as UDF. Each simulation was performed over 1200 seconds until the reaction reached a steady state. The calculations were using High Performance Computer (HPC) cluster at Purdue University Northwest. Detailed simulation parameters are listed in Table 2

3 Boundary and initial conditions

3.1 Computational domain

The computational geometry of the regenerator being studied is shown in Figure 1 (a). The regenerator cylindrical vessel includes nine two-stage cyclones, two levels of air rings, two spent catalyst inlets, and two regenerated catalyst outlets. The regenerator start-up operation normal starts with charging a certain amount of clean catalyst at the bottom. Fluidization air is then injected into the catalyst bed to form a fluidized bed. The continuous operation process then starts to recycle the spent catalyst from the riser reactor. The spent catalyst with a certain amount of transport air is fed into the regenerator through the spent catalyst inlets located at the bottom of the geometry. Air is continuously injected into the regenerator through the upper and lower air ring distributors located in the bottom to fluidize the catalyst bed and combust the coke on the catalyst surface. The catalysts carried by the gas to the top are separated from the gas in the two-stage cyclones and recycled back into the catalyst bed. This two stage group cyclones are generally equipped in FCC regenerators with the outlet duct of first stage cyclone directly coupled to the inlet duct of the secondary stage cyclone as shown in Figure 2. This group cyclones has advantages of high and flexible handling capacity, high efficiency, high separation precision and relatively low cost. [45,46] The regenerated catalysts are removed from the regenerator through the regenerated catalyst outlets with high temperature and recovered reactivity. A total number of 2 million cells was used for this simulation. The details of the mesh is shown in Figure 1(b). Mesh independent study can be found in previous work [39].

3.2 Operating conditions

Typical operational boundary conditions for this particular FCC regenerator was applied to the developed CFD model as shown in Table 3. The amount of regenerated catalyst extracted from

the regenerator is equal to the amount of spent catalyst input from the spent catalyst inlet. The walls were set as no-slip wall boundary conditions for both solid phase and gas phase. Each phase contains multiple species. According to the plant measurements, the catalyst used for this simulation contains 1 percent coke, with carbon count for 92% and the remaining 8% is hydrogen. The gas phase contains species O_2 , N_2 , CO , CO_2 , H_2O . In addition, the catalyst goes through the cyclone was defined 100% recycled back to the regenerators with all the species concentrations unchanged as shown in Figure 2, which was expressed by UDF. The simulation was conducted based on the initial startup condition.

3.3 Reaction mechanisms

The carbon and hydrogen combustion reactions were taken into consideration in this CFD model. The global reaction mechanisms, kinetics and heat generation are listed in Table 4. [47-49] The kinetic parameters for reaction1 (R1) and reaction 2 (R2) are obtained from the experimental work done by Kanervo et al. [47], in which reaction rates of combustion of coke on FCC solid catalyst particles to produce CO and CO_2 in a reactor were measured. The kinetic parameters from the experimental work of hydrogen combustion in carbonaceous deposits on zeolite-type cracking catalysts reported by Wang et al. [48] was used for the hydrogen combustion. The kinetics for the CO combustion is adopted from the work by Dryer and Glassman [49]. This kinetics does not include the effects CO combustion promoter which is used in the actual regenerator operations.

4 Results and discussions

4.1 Simulation results

The model has been validated by plant data under typical operation condition as shown in Table 5. The catalyst circulation flow rate through cyclones were predicted by the CFD model, which agrees with the real measurement data monitored in plant. Pressure drop between two locations at different heights (one in the dense zone and the other in the dilute zone) inside the regenerator is measured during the regenerator operation. The error of the pressure drop calculated by the model relative to the average of the pressure drop range of the actual regenerator is 4%. Temperature field and the major species volume fractions has also been compared with plant data. The relative errors between the temperature predicted by the model and measurements in

both dense zone and dilute zone are within 1%. The relative error of CO is high. However, it should be noted that the CO concentration at the cyclone inlets is extremely low. This high relative error of CO concentration is due to the fact that, the kinetics for the CO combustion used in the model does not take into account any CO combustion promoters. In the real operations, CO combustion promoters are added into the catalyst bed to promote CO combustion in the dense bed. It is desired to have as much CO as possible burned inside the dense bed thus the amount of CO that goes CO combustion in the dilute zone can be minimized. More detailed validation process can be found in previous work [39].

In this simulation, due to the transient flow properties, a transient simulation processes was applied to simulate fluid flow and combustion reactions which was started from initial startup condition to a quasi-steady state. The fluidization process of the solid FCC catalyst in the regenerator is shown in Figure 3.

Figure 3 shows that at the startup conditions, where the catalyst bed is resting at the bottom of the FCC regenerator. With the input of air from the air rings, the fluidization phenomenon took place. The catalysts were firstly fluidized by the air with a high fluidized bed due to the initial high accumulated momentum. After the flow reached a quasi-steady state after 100s, it shows similar flow patterns but different flow property values at specific locations over time. The catalyst solid volume fraction contour shows that there are four zones along the regenerator height: dense zone, sub-dense zone, dilute zone and sub-dilute zone. The sub-dense zone is also called the fluidized bed; while in the dense zone, the solid catalyst is difficult to be fluidized due to the geometry effect. Dilute zone has low catalyst concentration which is between the fluidized bed and cyclones. The region above the cyclones almost has no catalyst concentration which called sub-dilute zone as shown in Figure 3.

The fluidized bed combustion process also occurs with the development of fluid flow. The transient process of temperature evolution at five different normalized regenerator heights were plotted in Figure 4. The temperature value is the mass weighted average temperature on the cross sectional area.

Figure 4 shows the transient temperature evolution process inside a FCC regenerator. It is shown that the combustion occurs immediately after the spent catalysts are transported into the

regenerator. The gas temperature evolution inside the FCC reheating furnace can be divided into three stages. The gas temperature increases linearly at the first 200s. Then, the rate of temperature evolution increases dramatically from 300s to 600s. After 600s, the temperature increase rate reduces and reaches a steady state after 1000 seconds. In addition, among the five different levels, the level $h/H=0.15$ and $h/H=0.24$ are in the fluidized bed. The temperature evolution profiles at different heights indicate that the temperature in the fluidized bed is lower than temperature in the dilute phase and the maximum difference is approximately 20K. This temperature difference indicates a CO combustion occurred above the fluidized bed. At 1260s, after the flow and reaction reached quasi-steady state, the mass weighted average catalyst volume fraction and the temperature profiles along the FCC regenerator height were plotted in Figure 5.

Figure 5 shows that the average temperature in the fluidized bed is lower than that in the dilute zone. The transition region between the fluidized bed and the dilute zone raises the gas temperature due to the CO combustion. The spikes at the top region ($h/H=0.89$) on both the averaged solid volume fraction and temperature profiles are due to the effect of cyclone geometry. The catalyst accumulates on the cyclone top surface while the high temperature flue gas emits from the cyclones.

Figure 6 shows the mass weighted average mass fractions profiles of species $C_{<s>}$ and H_2 in the solid catalyst along the regenerator height after the flow reaching the quasi-steady state. It indicates that the mass fraction of $C_{<s>}$ and H_2 in the catalyst at the regenerated catalyst outlet are 0.09% and 0.0015%, respectively. By comparing to the original content 0.92% and 0.08%, the reduction rate for $C_{<s>}$ and H_2 after combustion are 90% and 98%, respectively. The $C_{<s>}$ and H_2 on the catalysts are further reduced in the dilute zone which increases the gas temperature at the dilute zone. The mass weighted average species concentrations in the gas phase along the regenerator height after reaction reached steady state are shown in Figure 7.

According to Figure 7, CO_2 , H_2O and O_2 are the major species, while the CO concentration is approximately zero. Along the regenerator height, the CO_2 mass fraction increases above the fluidized bed. O_2 mass fraction decreases greatly above the lower air ring, and further decreases

to a small percentage above the fluidized bed. Due to the fast hydrogen combustion, the H_2O mass fraction increases above the fluidized bed and remain stable below the cyclone.

4.2 Effect of oxygen enrichment

The ultimate goal for optimizing the existing FCC regenerator is to improve the FCC catalyst reactivity. Increasing the coke reduction without damaging the cyclone structure and catalyst itself by high temperature are the basic criteria for optimization. The optimal catalyst temperature in the dense is approximately 1000K. The simulation on FCC regenerator under the typical operating condition indicates that the coke reduction efficiency can be further improved. There are several parameters can be adjusted to improve the coke reduction: air flow rate, oxygen enrichment, geometry change. Oxygen enrichment is a technique that widely applied in the industrial furnace to improve combustion efficiency. Oxygen enrichment technique has been applied on current FCC regenerator operation process to improve the recovery of catalyst reactivity. Therefore, the effect of oxygen enrichment on the catalyst reactivity recovery process needs to be investigated based on the validated CFD model. The effect of 5% and 10% oxygen enrichment on the reaction inside the FCC regenerator has been studied. The effect of oxygen enrichment on the mass weighted average temperature field inside the FCC regenerator is shown in Figure 8.

According to Figure 8, 5% oxygen enrichment would increase approximately 6K in both the fluidized bed and the dilute zone along the FCC regenerator height. When further increase the oxygen enrichments to 10%, the average temperature increased approximately 2K in the dilute zone, which indicates that the combustion of the carbon and hydrogen in the solid phase reached a limit as shown in Figure 9.

According to Figure 9, with the increasing of oxygen enrichment, the mass weighted average carbon and hydrogen mass fractions in the fluidized bed decrease, which indicates an improvement in the reduction rates. The reduction rate of $C_{<s>}$ increases from 90% to 94.5% and the H_2 reduction rate increases from 98% to 99% when the oxygen enrichment is 5%. However, after oxygen enrichment exceeds 5%, the effect of oxygen enrichment on improving

carbon and hydrogen reactions is limited. The limitation is also indicated by the mass weighted average gas species plots in Figure 10.

According to Figure 10, with the increasing of oxygen enrichment, the CO_2 mass fraction increased in both fluidized bed and the dilute zone. The oxygen penetrates into in the bottom packed bed and increases the CO_2 mass fraction significantly. However, the CO_2 mass fraction stabilizes in the dilute phase when the oxygen enrichment exceeds 5%. Due to the fast reaction rate of hydrogen combustion, the oxygen enrichment has limited effect on the species H_2O distribution. It can be seen that with the increasing of oxygen enrichment, the mass fraction of H_2O increases at the normalized height around 0.3 where the transition between fluidized bed and dilute phase occurs. However, the H_2O mass fraction in the dilute zone keeps constant, which indicates that the hydrogen combustion occurred fast and oxygen enrichment effect is limited.

5 Conclusions

A three-dimensional multi-phase, multi-species reacting flow computational fluid dynamics (CFD) model has been established to simulate the flow characteristics and chemical reactions inside an FCC regenerator. The multiphase Eulerian model with kinetic theory of granular flow is employed. A modified drag model is used to calculate the drag force during solid catalyst fluidization process. Heterogeneous reaction model was employed where interphase reactions are considered. The finite-rate combustion model was used which use Arrhenius expressions. The developed CFD model was validated by using the plant data. This CFD model is able to predict the flow field, temperature distribution and species concentrations. The transient flow characteristics and the inter-phase reactions were studied. The effect of oxygen enrichment on the catalyst reactivity recovery was investigated, and the results show that coke reduction rate can be improved from 90% to 94.5% with 5% oxygen enrichment. The effect of oxygen enrichment is limited when it exceeds 5%. This simulation did not consider the CO combustion promoters, which could introduce errors on the CO concentration.

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7 Nomenclatures

a	absorption coefficient
C	linear-anisotropic phase function coefficient
CD	drag coefficient
dp	diameter of particle, m
dp^*	particle effective mean diameter in dense bed, 300 μ m
dp'	particle effective mean diameter in dilute phase, 150 μ m
T	temperature, K
T_{ip}	phase temperature
g	gravity acceleration, m/s ²
Y_i	species i mass fraction
g_O	radial distribution function
G	incident radiation
h	specific enthalpy
P	pressure, Pa
Re	Reynolds number
Nu	Nusselt number
Pr	Prandtl number
Rep^*	cluster Reynolds number

t	time, s
u	velocity, m/s
ρ_i	bulk density of phase i
V_{Fi}	volumetric fraction of phase i
MW_i	molecular weight of species i
ν_i	stoichiometric coefficient of reactants
T_{ref}	reference temperature (298K)
q	the heat flux
S	source term that includes sources of enthalpy
$h_{i,j}$	the intensity of heat exchange between gas and solid or liquid phase
$h_{i,p}$	the interphase enthalpy
K_g	the thermal conductivity of gas phase
v_g	the velocity of phase g
v_p	the velocity of phase p
m_{pg}	the mass transfer from p phase to g phase
S_q	the source term
u_g	superficial gas velocity, m/s
u_p	superficial particle velocity, m/s
I	unit stress tensor

Greek letters

α	volume fraction
β	inter-phase momentum exchange coefficient, kg/m ³ -s
γ	collisional dissipation of energy fluctuation, kg-s ³ /m

Γ_{dil}	dilute diffusion coefficient for energy fluctuation, kg-s/m
Γ	diffusion coefficient for the energy fluctuation, kg-s/m
Θ	granular temperature, m ² /s ²
μ_p	particle phase shear viscosity, Pa-s
μ_g	gas phase shear viscosity, Pa-s
λ_p	solid bulk viscosity, Pa-s
λ_g	gas bulk viscosity, Pa-s
ρ	density, kg/m ³
τ	stress tensor, Pa
e	the coefficient of restitution, 0.9
σ_s	scattering coefficient
k	reaction rate constant

Superscripts and Subscripts

i,j,k	direction coordinate
g	gas phase
max	maximum
p	particle phase
NR	total number of reactants

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List of Tables

Table 1 Modified drag coefficient with zone classification

Table 2 Simulation parameters

Table 3 Boundary Conditions

Table 4 Reaction mechanisms and kinetics

Table 5 Relative errors of the simulation results when compared with plant data

Table 1 Modified drag coefficient with zone classification

Void fraction	Drag force model	Drag force coefficient
≤ 0.80	Ergun[40]	$\beta_1 = 150 \frac{\alpha_p(1 - \alpha_g)\mu_g}{\alpha_g(d_p^*)^2} + 1.75 \frac{\rho_g \alpha_p \vec{u}_p - \vec{u}_g }{d_p^*}$
0.8-0.933	ZP	$\beta_2 = \frac{5}{72} C_D \frac{\alpha_p \alpha_g \rho_g \vec{u}_p - \vec{u}_g }{d_p^* (1 - \alpha_g)^{0.293}}$ $C_D = \begin{cases} \frac{24}{\alpha_g Re_p^*} (1 + 0.15 (\alpha_g Re_p^*)^{0.687}) & (Re_p^* \leq 1000) \\ 0.44 & (Re_p^* \geq 1000) \end{cases}$ $Re_p^* = \frac{\rho_g d_p^* \vec{u}_g - \vec{u}_p }{\mu_g}$
0.933-0.990	Wen& Yu[41]	$\beta_3 = \frac{3}{4} C_D \frac{\alpha_p \alpha_g \rho_g \vec{u}_p - \vec{u}_g }{d_p'} \alpha_g^{-2.65}$ $C_D = \frac{24}{\alpha_g Re_p'} (1 + 0.15 (\alpha_g Re_p')^{0.687})$ $Re_p' = \frac{\rho_g d_p' \vec{u}_g - \vec{u}_p }{\mu_g}$
0.990-1.00	Schiller& Naumann[42]	$\beta_4 = \frac{3}{4} C_D \frac{\alpha_g \alpha_p \rho_g \vec{u}_p - \vec{u}_g }{d_p'}$ $C_D = \begin{cases} \frac{24}{Re_p'} (1 + 0.15 Re_p'^{0.687}) & (Re_p' \leq 1000) \\ 0.44 & (Re_p' \geq 1000) \end{cases}$ $Re_p' = \frac{\rho_g d_p' \vec{u}_g - \vec{u}_p }{\mu_g}$

Table 2 Simulation parameters

Parameters	Value and methods
Gas-solid two phase flow model	Eulerian-Eulerian model with kinetic theory (granular)
Solver	Pressure based and transient
Flow type	Laminar
Wall boundary condition	No slip
Time step used	0.01s
Pressure velocity coupling scheme	Phase Coupled SIMPLE
Under-relaxation Factors	Pressure 0.3, momentum 0.7, volume fraction 0.5, granular temperature 0.2. Species 0.6
Maximum solid packing volume fraction	0.6
Spatial Discretizations	Gradient: Green-Gauss Cell Based Momentum, energy, species: second order upwind, Volume fraction: first order upwind.
Gas mixture density	Incompressible ideal gas law.
Superficial velocity	0.6~0.7m/s
Absorption coefficient	Gray WSGG with domain based mean beam length
Scattering coefficient	0
Solid mixture density	Volume weighted mixing law
Catalyst particle density	1440 kg/m ³
Catalyst particle mean diameter	75µm
Solid particle absorption efficiency	0.9
Solid particle scattering efficiency	0.1

Table 3 Boundary Conditions

	Spent Catalyst Inlet	Upper Air Ring	Lower Air Ring	Regenerated Catalyst Outlet
Velocity (m/s)	5.6	12.9	15.7	1.1
Gas volume fraction	0.05	1	1	0
Solid volume fraction	0.95	0	0	1

Table 4 Reaction mechanisms and kinetics

	<i>Reactions</i>	<i>Heat of reaction (kJ/mol)</i>	<i>Pre-exponential factor</i>	<i>Activation Energy (J/mol)</i>
R1	$C + \frac{1}{2} O_2 \rightarrow CO$	118	$0.155 \times 10^8 \text{ s}^{-1} \cdot \text{atm}^{-1}$	159,000
R2	$C + O_2 \rightarrow CO_2$	403	$0.376 \times 10^8 \text{ s}^{-1} \cdot \text{atm}^{-1}$	110,000
R3	$CO + \frac{1}{2} O_2 \rightarrow CO_2$	283	$0.149 \times 10^{12} \text{ kg}^{-1} \cdot \text{m}^{-3} \cdot \text{atm}^{-2}$	212,000
R4	$H_2 + \frac{1}{2} O_2 \rightarrow H_2O$	600	$3.3 \times 10^{07} \text{ kg}^{-1} \cdot \text{s}^{-1} \cdot \text{atm}^{-1}$	157,700

Table 5 Relative errors of the simulation results when
compared with plant data

<i>Parameters</i>	<i>Relative error</i>
Catalyst circulation	2.74%
ΔP (inH ₂ O)	4.0%
Dense zone temperature	0.50%
Dilute zone temperature	0.29%
C reduction rate (%)	1.7%
<u>Volume fraction at outlets:</u>	
CO (ppm)	8881.8%
CO ₂	1.2%
O ₂ (vol%)	14.9%

List of Figures

Figure 1 (a).Computational domain with boundaries, (b). mesh

Figure 2 Cyclone boundary conditions

Figure 3 Solid volume fraction profiles changing with time

Figure 4 Gas temperature evolution at different levels along the regenerator height

Figure 5 Mass weighted average solid volume fraction and gas temperature along regenerator height

Figure 6 Mass weighted average species mass fraction in solid phase along regenerator height

Figure 7 Mass weighted average species mass fractions in gas phase along regenerator height

Figure 8 Effect of oxygen enrichments on average gas temperatures along regenerator height

Figure 9 Effect of oxygen enrichments on species $C_{<s>}$ and H_2 in the solid phase along the regenerator height

Figure 10 Effect of oxygen enrichments on gas phase species CO_2 and H_2O along the regenerator height

(a)

(b)

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