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Validation and application of CPFD models in simulating hydrodynamics and reactions in riser reactor with Geldart A particles

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ABSTRACT

A Computational Particle Fluid Dynamics (CPFD) model, which has the ability of revealing the coupled flow-reaction behaviors on the scales ranging from an individual particle to the whole reactor, was developed for studying the gas-solids circulating fluidized bed (CFB) riser reactor handling Geldart A particles. The model was validated against available experimental data with respects to the hydrodynamics (e.g. distributions of solids holdup and solids velocity) and the reaction behaviors (e.g. distribution of ozone concentration for ozone decomposition), and acceptable agreements were achieved between the modeling results and the experimental data. The CPFD model was further extended for analyzing the gas-solids flow hydrodynamics and the cracking reactions in an industrial Fluid Catalytic Cracking (FCC) riser reactor. Modeling results indicate that the volume of gas in the CFB riser will vary due to the presence of interphase chemical reactions (e.g. catalytic cracking reactions in FCC), which can significantly influence the gas-solids flow hydrodynamics. It was demonstrated that the CPFD model can be applied to quantify the relationship between the flow hydrodynamics and the chemical reactions in multiphase flow-reaction systems.

1. Introduction

Circulating fluidized beds (CFB) with fine Geldart A particles have been widely applied in various industrial processes, e.g. FCC process in refinery, coal combustion, etc. The performance of the CFB is closely related to the complex gas-solids flow hydrodynamics and reaction characteristics inside the CFB riser reactor, which has attracted extensive academic researches through the world [1]. Owning to its advantages of efficiency, convenience and low-cost and its ability in providing more comprehensive and crucial information [2], the Computational Fluid Dynamics (CFD) has gradually become a reliable and effective tool for troubleshooting, designing and scaling-up [3] of the CFB riser through investigating the complex hydrodynamics and reaction characteristics inside the CFB riser.

In most of previous CFD simulations, both Eulerian-Eulerian two-fluid model (TFM) [4] and Eulerian-Lagrangian discrete element model (DEM) [5] have been used for studying gas-solids fluidized beds [6,7]. Despite that the TFM model treating gas and solid phases as two interpenetrating continua can deal with large-scale industrial systems, it cannot accurately consider the realistic characteristics of particles. Due to the pseudo-fluid rheological properties of solid phase especially for fine Geldart A particles [8], the reliability and accuracy of some of the empirical relations for describing the strong interparticle forces [9,10], including interfacial friction, shear stress, and cohesive force, are still in dispute in the TFM, which is a limitation of the TFM. In contrast, the DEM model can individually track each particle by solving the Newton equation [11,12], which indicates that the detailed particle flow behaviors in fluidized beds can be predicted in DEM [13]. However, the huge computational requirements of DEM in describing dense particle-particle interactions are proportional to the number of particles simulated [13], which makes it difficult for the DEM in describing a large-scale industrial CFB riser with billions of particles [14].

Currently, in order to overcome the limitations of TFM and DEM, the CPFD model, which is based on multi-phase particle in cell (MP-PIC) method and is in Eulerian-Lagrangian scheme, proposed by Snider and his colleagues [15] has been applied to simulate gas-solids fluidized beds through defining the concept of 'parcel of particles'. Each computational parcel contains a number of particles with identical properties such as density, volume, size, shape and velocity. Due to its unique feature, the CPFD method is capable of simulating large commercial CFB risers containing billions of particles by applying millions of computational parcels [6], and it can serve as a candidate to achieve quick and efficient simulation of industrial gas-solids systems.

Chen et al. [6] studied the applicability of the CPFD method for simulating gas-solids flow hydrodynamics in a CFB riser containing Geldart A particles. They indicated that the drag forces calculated by the conventional drag model including Wen-Yu model, Ergun model, Wen-Yu/Ergun model and Turton model in the CPFD method overestimated

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Table 1
Detailed governing equations in the simulation.

Fluid phase continuity equation

$$\frac{\partial \theta_f \rho_f}{\partial t} + \nabla \cdot (\theta_f \rho_f u_f) = 0 \quad \text{(T1-1)}$$

Gas phase momentum equation

$$\frac{\partial(\theta_f \rho_f u_f)}{\partial t} + \nabla \cdot (\theta_f \rho_f u_f u_f) = -\theta_f \nabla P + \theta_f \mu_f \nabla^2 u_f + \theta_f \rho_f g - F \quad \text{(T1-2)}$$

Momentum exchange between gas and particle phases

$$F = \iiint f V_p \rho_p \left[D(u_f - u_p) - \frac{1}{\rho_p}\nabla p\right] dV_p d\rho_p du_p \quad \text{(T1-3)}$$

Liouville equation for finding particle positions

$$\frac{\partial f}{\partial t} + \nabla(f u_p) + \nabla_{u_p}(fA) = 0 \quad \text{(T1-4)}$$

Particle acceleration

$$A = D(u_f - u_p) - \frac{1}{\rho_p}\nabla p + g - \frac{1}{\theta_p \rho_p}\nabla \tau_p \quad \text{(T1-5)}$$

Particle normal stress model

$$\tau_p = \frac{P_s \theta_p^{\beta}}{\max[(\theta_{cp} - \theta_p), \varepsilon(1 - \theta_p)]} \quad \text{(T1-6)}$$

Particle volume fraction in each cell

$$\theta_p = \iiint f V_p dV_p d\rho_p du_p \quad \text{(T1-7)}$$

Drag model (Gidaspow model)

$$C_d = \frac{24}{\mathrm{Re}}\theta_f^{-2.65} \qquad (\mathrm{Re} < 0.5) \quad \text{(T1-8)}$$

$$C_d = \frac{24}{\mathrm{Re}}(1 + 0.15\ \mathrm{Re}^{0.687})\theta_f^{-2.65} \qquad (0.5 \le \mathrm{Re} \le 1000) \quad \text{(T1-9)}$$

$$C_d = 0.44\theta_f^{-2.65} \qquad (\mathrm{Re} > 1000) \quad \text{(T1-10)}$$

$$D_1 = 0.75 C_d \frac{\rho_f}{\rho_p}\frac{|u_f - u_p|}{d_p} \quad \text{(T1-11)}$$

$$\mathrm{Re} = \frac{\rho_f d_p |u_f - u_p|}{u_f} \quad \text{(T1-12)}$$

$$D_2 = \left(\frac{180\theta_p}{\theta_g\ \mathrm{Re}} + 2\right)\frac{\rho_f}{\rho_p}\frac{|u_f - u_p|}{d_p} \quad \text{(T1-13)}$$

$$D = D_1 \qquad (\theta_p < 0.75\theta_{cp}) \quad \text{(T1-14)}$$

$$D = \frac{\theta_p - 0.85\theta_{cp}}{0.85\theta_{cp} - 0.75\theta_{cp}}(D_2 - D_1) + D_1 \qquad (0.75\theta_{cp} \le \theta_p \le 0.85\theta_{cp}) \quad \text{(T1-15)}$$

$$D = D_2 \qquad (\theta_p > 0.85\theta_{cp}) \quad \text{(T1-16)}$$

Drag model (EMMS model)

$$\beta = \frac{3}{4} C_D \frac{\varepsilon_p \varepsilon_f \rho_f |u_f - u_p|}{d_p} H_D \quad \text{(T1-17)}$$

$$C_D = \frac{24(1 + 0.15\ \mathrm{Re}_p^{0.678})}{d_p} \qquad (\mathrm{Re}_p < 1000) \quad \text{(T1-18)}$$

$$C_D = 0.44 \qquad (\mathrm{Re}_p \ge 1000) \quad \text{(T1-19)}$$

$$\mathrm{Re}_p = \frac{\varepsilon_f \rho_f |u_f - u_p| d_p}{u_f} \quad \text{(T1-20)}$$

$$H_D = a(\mathrm{Re}_p + b)^c \quad \text{(T1-21)}$$

For the CFB riser under Gs = 200 kg/(m^2·s), Ug = 7 m/s

$$a = \begin{cases} \exp\left(0.5120 + 471.7406{\varepsilon_f}^{2.5} + 116.8694\frac{\varepsilon_f}{\ln \varepsilon_f}\right) & 0.457 \le \varepsilon_f < 0.8 \\ \frac{1}{\left(0.5690 + 11201.4430\ \ln^2 \varepsilon_f - \frac{0.0001868}{\ln \varepsilon_f}\right)} & 0.8 \le \varepsilon_f < 0.9997 \\ 1 & 0.9997 \le \varepsilon_f < 1 \end{cases} \quad \text{(T1-22)}$$

$$b = \begin{cases} \frac{\varepsilon_f}{(-0.05570\exp(-\exp(92.9004 - 209.2822\varepsilon_f)))} + 9.4089 & 0.457 \le \varepsilon_f < 0.48 \\ -0.8456\exp(-\exp(141.1489 - 281.1403\varepsilon_f)) + 0.8560 & 0.48 \le \varepsilon_f < 0.6 \\ -0.001343\exp\left(\frac{(\ln \varepsilon_f + 0.2708)^2}{0.01890}\right) + 0.06095 & 0.6 \le \varepsilon_f < 0.98 \\ 0.6141 - 0.5982\exp(-361.6032{\varepsilon_f}^{1177.6292}) & 0.98 \le \varepsilon_f < 0.9997 \end{cases} \quad \text{(T1-23)}$$

$$c = \begin{cases} \frac{0.5498}{\left((1 + \exp(23.4547 - 44.0615\varepsilon_f))^{\frac{1}{0.3682}}\right)} & 0.457 \le \varepsilon_f < 0.622 \\ 0.9387 - 0.3931{\varepsilon_f}^{63.0517} - 0.4291\exp(\varepsilon_f) + \frac{0.6075}{{\varepsilon_f}^{-0.9801}} & 0.622 \le \varepsilon_f < 0.9997 \\ 0 & 0.9997 \le \varepsilon_f < 1 \end{cases} \quad \text{(T1-24)}$$

For the CFB riser under Gs = 300 kg/(m^2·s), Ug = 7 m/s

$$a = \begin{cases} \exp\left(-14.5750 + 312.7533{\varepsilon_f}^2 + \frac{88.8204\varepsilon_f}{\ln \varepsilon_f}\right) & 0.457 \le \varepsilon_f < 0.8 \\ \frac{2.1671}{\left(1.6348 + \left(\frac{\varepsilon_f - 0.9975}{0.004877}\right)^2\right)} + 0.01925 & 0.8 \le \varepsilon_f < 0.9997 \\ 1 & 0.9997 \le \varepsilon_f < 1 \end{cases} \quad \text{(T1-25)}$$

$$b = \begin{cases} 335829.8019 - 58503.7150{\varepsilon_f}^2 - 346197.6827\frac{\ln \varepsilon_f}{\varepsilon_f} - \frac{283243.1637}{{\varepsilon_f}^{1.5}} & 0.457 \le \varepsilon_f < 0.48 \\ -0.9062\exp\left(-\exp\left(\frac{\varepsilon_f - 0.4937}{-0.003305}\right)\right) + 0.9105 & 0.48 \le \varepsilon_f < 0.6 \\ -0.05969{\varepsilon_f}^{44.1159} - 0.01195{\varepsilon_f}^{-2.006296} + 0.0490 & 0.6 \le \varepsilon_f < 0.98 \\ 0.6151 - 0.6007\exp(-347.2199{\varepsilon_f}^{1193.8833}) & 0.98 \le \varepsilon_f < 0.9997 \end{cases} \quad \text{(T1-26)}$$

$$c = \begin{cases} \frac{0.5657}{\left(\left(1 + \exp\left(-\frac{(\varepsilon_f - 0.5229)}{0.02132}\right)\right)^{2.7843}\right)} & 0.457 \le \varepsilon_f < 0.622 \\ \exp\left(-0.7954 + \frac{0.1090}{\ln(\varepsilon_f)} + \frac{0.1300}{\varepsilon_f}\right) & 0.622 \le \varepsilon_f < 0.9997 \\ 0 & 0.9997 \le \varepsilon_f < 1 \end{cases} \quad \text{(T1-27)}$$

For the industrial FCC riser

$$a = \begin{cases} \exp\left(6.9292 + 588.5260{\varepsilon_f}^{2.5} + \frac{154.9300\varepsilon_f}{\ln \varepsilon_f}\right) & 0.4 \le \varepsilon_f < 0.8 \\ \frac{0.01789}{0.01418 + \left(\frac{\varepsilon_f - 0.9975}{0.04471}\right)^2} + 0.01863 & 0.8 \le \varepsilon_f < 0.9997 \\ 1 & 0.9997 \le \varepsilon_f < 1 \end{cases} \quad \text{(T1-28)}$$

$$b = \begin{cases} 731763.7904 - 340361.2073\varepsilon_f - \frac{943439.1025}{\varepsilon_f} + \frac{659574.2703}{{\varepsilon_f}^{1.5}} - 135074.8485{\varepsilon_f}^2 & 0.4 \le \varepsilon_f < 0.46 \\ 1.3451\exp(-\exp(-37.9801 + 83.8802\varepsilon_f)) + 0.01152 & 0.46 \le \varepsilon_f < 0.53 \\ -27.9991 + 143.2336\varepsilon_f - 270.8919{\varepsilon_f}^2 + 226.7026{\varepsilon_f}^3 - 71.04820{\varepsilon_f}^4 & 0.53 \le \varepsilon_f < 0.95 \\ 0.3866{\varepsilon_f}^{-460.5608 - 96249.5800\ \ln \varepsilon_f} - 2.03795\ \ln \varepsilon_f & 0.95 \le \varepsilon_f < 0.9997 \end{cases} \quad \text{(T1-29)}$$

$$c = \begin{cases} \frac{1}{2.8217\varepsilon_f(1 + 33700572.3662\exp(-31.7864\varepsilon_f))} & 0.4 \le \varepsilon_f < 0.95 \\ 0.06891 + 0.2873\exp(-8.5327{\varepsilon_f}^{201.008284}) & 0.95 \le \varepsilon_f < 0.9997 \\ 0 & 0.9997 \le \varepsilon_f < 1 \end{cases} \quad \text{(T1-30)}$$