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A model for improving the Euler–Euler two-phase flow theory to predict chemical reactions in circulating fluidized beds

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ABSTRACT

In this paper, a model of predicting the reaction in CFB was developed by coupling some developed sub-grid models into the Euler–Euler two-phase flow model (TFM) with the relatively coarse mesh. In this model, the local heterogeneous flow structural parameters were obtained by solving the momentum and mass conservation equations and using some widely accepted semi-empirical equations, for example, the well-known Ergun and Richardson-Zaki equation. The heterogeneous fluid flow was resolved by coupling the momentum transfer coefficient based on the local heterogeneous structural parameters into the TFM model. The gas-solid mass transfer coefficient in terms of the local heterogeneous fluid flow was obtained in the assumed process, which was completely dominated by the gas-solid mass transfer. And then, the reaction was predicted by solving the balance equation between the mass transfer and chemical reaction. This method improves the general applicability of developed model and reduces the calculating process, and which has been verified by the ozone decomposition reaction in CFB from the literature.

1. Introduction

Circulating fluidized beds (CFBs) are prevalent in many chemical engineering applications, for example, fluid catalytic cracking (FCC) in the oil process, ethylene polymerization, coal gasification and combustion, and mineral reducing or oxidizing roasting as their performance in gas–solid mass/heat transfer is good and reliable. In order to meet the requirements of different chemical reactions, the developer had to optimize the geometrical structure to tailor the fluid dynamics, back mixing, heat and mass transfers by the experimental and theoretical analysis [1–4]. Due to the lack of relevant quantitative information, optimizing the reactor structure and determining the optimum and safe operating conditions of the relevant process has to mainly depend on the numerous experimental results from the laboratory test to the pilot-scale plants, which would spend a great number of labor power and material resource and slow the process of commercializing new reaction. Therefore, up to now, reducing the number of experiment based on accurately modeling the reaction in the different reactors still attracts many researchers and engineers' attentions. The general conclusion in literature shows that resolving the fluid flow and accurately predicting the mass and heat transfer are critical for obtaining the detailed information for designing a CFB to perform a new reaction. Due to the low performance of digital computers in the last, the heterogeneous fluid flow in CFB was often simplified as a plug flow (PF) or continuously stirred tank (CST) [5]. The mass and heat transfer were predicted by the dimensionless parameters from correlating the experimental data, for example, the back-mixing (Péclet number) [6], heat transfer [7] (Nusselt number) and mass transfer coefficient (Sherwood number) [8–10]. However, due to the over simplification of heterogeneous fluid flow and the limited valid range of dimensionless parameters, a relatively larger safety factor has to be used in designing a new CFB reactor based on these simple and semi-empirical models. Therefore, some efforts still need to be directed to develop some accurate and general models to accurately predict the reaction.

The development of computational fluid dynamics (CFD) [11] enables the effects of fluid flow on the performance of reactions in the complex reactor hardware to investigate in the greater detail by using the numerical simulations. From a theoretical viewpoint, most of the fluid flow in CFB can be predicted by refining the calculating mesh and employing the appropriate turbulent models [12]. In practice, the compromises have to be made between the consumption of computational resources and the reliability of information obtained in analyzing the industrial reactors. The relatively coarse calculation mesh and simple Euler–Euler two-flow models (TFM) had to be employed to reduce the computation cost. Unfortunately, the natural features of heterogeneous fluid flow in CFB cannot be captured by this kind of

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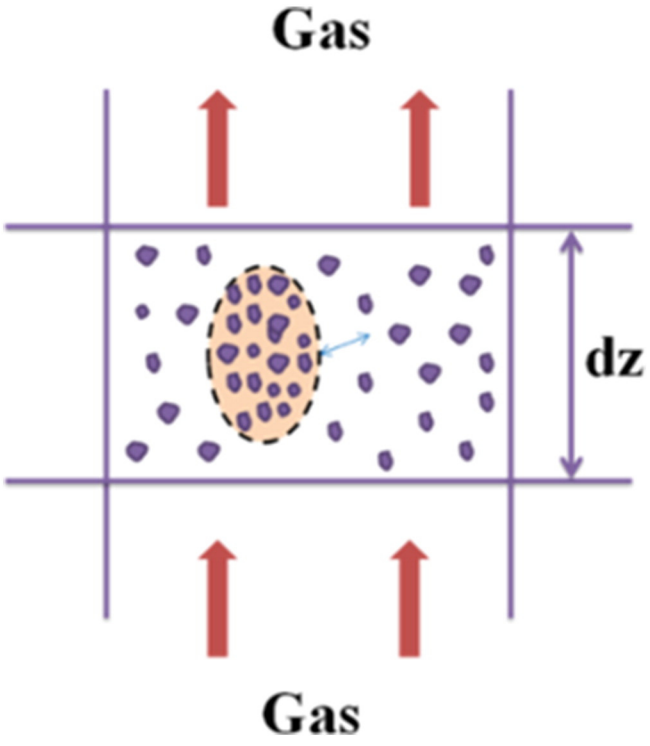

Fig. 1. Heterogeneous flow structure in a calculation mesh grid.

model, for example, in the core-annulus flow structure with being dilute at the center and dense at the wall, and the S-type axial distribution with being dilute in the upper part and dense in the lower part [13]. An efficient method of improving the low-resolution of TFM models is to couple some sub-grid constitutive relations, for example, the filtered two-fluid model (FTFM) developed by Sundaresan's group [14–16], and the energy minimization multi-scale (EMMS) model developed by Li's group [17,18]. All simulation results showed that these sub-grid models could improve the accuracy of TFM and capture the natural heterogeneous features of the radial and axial distributions of voidage.

Another main parameter for predicting the reaction in CFB is the gas-solid mass transfer. The mass transfer coefficient can be evaluated by the dimensionless Sherwood number, which only depends on the information of fluid flow. In the last, the relevant calculating expressions were obtained by correlating the experimental data in the packed bed or fluidized bed. However, due to the effect of various operational conditions and heterogeneous fluid flow, the values of mass transfer coefficient in CFB were widely dispersed in the range from 10^{-2} to 10^{5} in literature [19,20]. Until now, there is still no generally accepted answer to the question of how to select an appropriate equation to evaluate the dimensionless Sherwood number in a CFB. Some researchers [21,22] also tried to use the TFM model to predict the mass transfer, when the heterogeneous fluid flow was resolved by coupling the developed sub-grid drag model into the TFM model. The simulating results showed that the mass transfer coefficient was still overestimated because the influence of meso-scale cluster was not considered. Gao et al. [23,24] firstly considered this kind of effect to predict the relevant mass transfer coefficient in CFB by replacing the particle catalyst diameter in Jung–La Nauze's equation with the cluster diameter. This method depended on the assumption that the catalyst just on the surface of cluster was valid in CFB, which has not been validated by any theoretical and experimental results in the literature. Another method was the EMMS/mass model developed by Dong [19,25]. In their model, the mass transfer coefficient in each pseudo-phase was calculated by the dimensionless Sherwood number in the literature. From a theoretical viewpoint, this method was acceptable because the dilute and dense phase was assumed to be homogeneous in the EMMS model [20], which was consistent with the relevant experimental condition of correlating the dimensionless

Table 1
Governing equations for two-fluid model and its constitutive relations.

Continuity equation

$$\frac{\partial(\varepsilon_k\rho_k)}{\partial t}+\nabla(\varepsilon_k\rho_k u_k)=0$$

Momentum equation (k = g,s)

$$\frac{\partial(\varepsilon_k\rho_k u_k)}{\partial t}+\nabla(\varepsilon_k\rho_k u_k u_k)=-\varepsilon_k\nabla P_g+\varepsilon_k\rho_k g+\nabla\tau_k+\beta(u_s-u_g)$$

Gas phase stress

$$\tau_g=2\mu_g S_g$$

Solid phase stress

$$\tau_s=(-p_s+\lambda_s\nabla\mu_s)\delta+2\mu_s S_s$$

Deformation rate

$$S_k=\frac{1}{2}\left[\nabla u_k+(\nabla u_k)^T\right]-\frac{1}{3}\nabla u_k\delta$$

Solid phase pressure

$$p_s=\varepsilon_s\rho_s\Theta[1+2(1+e)\varepsilon_s g_0]$$

Solid phase shear viscosity

$$\mu_s=\frac{4}{3}\varepsilon_s{}^2\rho_s d_p g_0(1+e)\sqrt{\frac{\Theta}{\pi}}+\frac{2\mu_{s,dilute}}{(1+e)g_0}\left[1+\frac{4}{5}(1+e)\varepsilon_s g_0\right]^2$$

$$\mu_{s,dilute}=\frac{5}{96}\rho_s d_p\sqrt{\pi\Theta}$$

Radial distribution functions

$$g_0=\left[1-\left(\frac{\varepsilon_g}{\varepsilon_{sm}}\right)^{1/3}\right]^{-1}$$

Granular temperature equation

$$\frac{3}{2}\left[\frac{\partial(\varepsilon_s\rho_s\Theta)}{\partial t}+\nabla(\varepsilon_s\rho_s u_s\Theta)\right]=\tau_s:\nabla u_s-\nabla q-\gamma+\beta\overline{C_g C}-3\beta\Theta$$

Collisional energy dissipation

$$\gamma=3(1-e^2)\varepsilon_s{}^2\rho_s g_0\Theta\left[\frac{4}{d_p}\sqrt{\frac{\Theta}{\pi}}-\nabla u_s\right]$$

Flux of fluctuating energy

$$q=-k\nabla\Theta$$

Conductivity if the fluctuating energy

$$k=\frac{2k^k\left[1+\frac{6}{5}(1+e)\varepsilon_s g_0\right]^2}{(1+e)g_0}+k^c$$

$$k^k=\frac{75}{384}d_p\rho_s\sqrt{\Theta\pi}$$

$$k^c=2\varepsilon_s{}^2\rho_s d_p(1+e)g_0\sqrt{\frac{\Theta}{\pi}}$$

Drag coefficient Eq.(1)