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Optimal design of a wet-type desulphurization absorber by the numerical simulation method

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ABSTRACT

Numerical study of gas–liquid flow in a wet-type desulphurization absorber is presented and the influences of different inlet and deflector structures on the device performance are identified for optimizing its structure. The dependability of numerical model is validated by the good agreement between the measured and predicted results. Besides, the results of droplet trajectories analyzed by the mechanical formulas are consistent with the simulation results as well. The performance of gas flow field is affected significantly by the inlet structures. The main reason for uneven distribution of liquid-phase is the first layer deflector rather than the gas flow. After removing the first layer deflector, the mass percentage distribution of liquid-phase in the near-wall region is reduced from 68–87% to 25–40%. The temperature distribution and relative humidity depend largely on the distribution of liquid-phase and the gas flow field. Optimized structures improve the pressure drop of device.

Keywords: Structural optimization; Two-phase flow; Temperature distribution; Liquid-phase distribution; Numerical simulation; Eulerian–Lagrangian model

1. Introduction

Air pollution, which is caused by SO_2 and dust derived from the fossil fuel combustion, has received more and more attention (Marocco, 2010; Brogren and Karlsson, 1997) recently. Especially in China, the national emission standards of air pollutants of thermal power plants are becoming increasingly stringent. For instance, the concentration of SO_2 emissions is changed from 400–1200 mg/m^3 (GB 13223-2003) to 100–400 mg/m^3 (GB 13223-2011), and the concentration of dust emission is also changed from 50–600 mg/m^3 (GB 13223-2003) to 30 mg/m^3 (GB 13223-2011). However, the traditional purification devices cannot meet the strict requirement of these limitations. Therefore, the updates of purification devices are extremely urgent. The PCF (Chinese LOGO) device is a well proven absorber of wet flue gas desulphurization (WFGD) in industrial application. With high purification efficiency, low pressure drop and perfect performance of dehydration, the PCF device is widely installed in China (Gao et al., 2010). But the unreasonable local structures make the flue gas, liquid-phase and temperature distribute unevenly in the reaction zone, which is not conducive to the mass transfer between gas and liquid in the PCF device (Tao, 2001; Dou et al., 2009). In order to further improve the purification efficiency of the PCF device, this paper presents a study of the structural optimization using CFD method to regulate the gas flow field and liquid-phase distribution.

In view of shortening development cycles and reducing development cost, it is very important to assess the performances of different setups and to confirm the influences of different design parameters in the early stages (Nova et al., 2006). In those respects, the use of numerical simulation is a key factor. In the past two decades, significant progress has been made in the mathematical model of the wet flue

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gas desulfurization (WFGD) based on computational fluid dynamics (CFD) (Delgadillo and Rajamani, 2005; Launder and Spalding, 1972; Josserand and Zaleski, 2003; Rhodes et al., 2001). And abundant investigators employed CFD method to evaluate the performances of the hydrocyclone, fluidization bed and WFGD devices and then optimize the structural designs of them (Bernardo et al., 2006; Lu et al., 2007; Li et al., 2008; Wang and Yu, 2006). Furthermore, Nowakowski et al. (2004) elaborated the accuracy of numerical simulation and pointed out that the utilizing of numerical results in device design is advisable and promising. Comparing with the standard k–ε turbulence model which is not suitable for flow with high mean shear rate or material separation (Hoekstra et al., 1999; Wang et al., 2006), the Realizable k–ε turbulence model is more appropriate for anisotropic turbulence (Shih et al., 1995; Wang, 2004) and has been increasingly concerned in the studies of flow characteristics of the desulfurization towers (Marocco and Inzoli, 2009; Xua et al., 2013). Although the most accurate model for anisotropic turbulence is Reynolds stress model (RSM), it has the disadvantage of being more computationally expensive (Pant et al., 2002; Wang et al., 2006). Therefore, Marocco and Inzoli (2009) and Shih et al. (1995) chose the realizable k–ε turbulence model in their simulation studies and the simulation results were consistent with the experimental results very well.

Gas–liquid two-phase flow in the desulfurization tower can be simulated using the Eulerian–Eulerian and Eulerian–Lagrangian approaches (Ashraf Ali and Pushpavanam, 2011; Lu et al., 2008; Hajidavalloo et al., 2013), but the accuracy of Eulerian–Eulerian approach relies heavily on empirical constitutive equations and the effects of particle size, particle agglomeration and breakup cannot be fully taken into account (Berlemont et al., 1998; Marocco, 2010). The Eulerian–Lagrangian model, however, involves less empirical equations and is more suitable for providing detailed information of the discrete phase. Furthermore, the heat transfer between gas and liquid phase can be also taken into account easily (Marocco and Inzoli, 2009; Narasimha et al., 2005). Hence, generally, the fluid dynamics of gas–liquid phase inside the wet desulfurization tower is modeled with the Euler–Lagrange approach if the volume fraction of discrete phase is less than 10% (Buwa et al., 2006). In Eulerian–Lagrangian approach, the continuous phase is modeled in Eulerian framework (Zhang and Ahmadi, 2005), while the discrete phase is modeled with Lagrangian approach by tracking a large number of particles through the computational domain (Nowakowski et al., 2004).

Compared with experimental method, numerical simulation method is more convenient, less costly and easier to evaluate the overall performances of the device (Wang and Yu, 2006). Therefore, the gas–liquid two-phase flow in the PCF device was studied by the CFD software package (ANSYS-FLUENT) (Marocco, 2010; Jiao et al., 2006). The numerical simulations were run in a processor Xeon with 8GB RAM and every simulation took approximately 50 h. The Realizable k–ε turbulence model, the Eulerian–Lagrangian model and the SIMPLEC algorithm (Van Doormal and Raithby, 1984) were appropriately applied in these numerical simulations. The simulations focused on the influences of different inlet and deflector structures on the gas flow field, liquid-phase distribution, temperature distribution and the pressure drop. Additionally, the experiments and theoretical analyses using the Newton's second law were carried out to confirm and support the simulation results.

2. Governing equations

2.1. Carrier phase

For modeling the gas flow field in the PCF device, the incompressible Reynolds average Navier–Stokes (RANS) equations are supplemented by the realizable k–ε turbulence model. The effect of particle known as turbulence modulation is neglected due to the weak of it for low volume droplets concentration. Therefore the realizable k–ε turbulence model is used in its formulation for single-phase flows (Shih et al., 1995) and the Reynolds stress tensor is related to the average velocity gradient and turbulent viscosity of the flow following Boussinesq assumption (Marocco and Inzoli, 2009). The following equations describe the steady-state conservation equations of mass, momentum, energy and species mass, respectively:

$$\frac{\partial}{\partial x_i}(\rho_g \bar{u}_i) = 0 \tag{1}$$

$$\frac{\partial}{\partial x_j}(\rho_g \bar{u}_i \bar{u}_j) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu \frac{\partial \bar{u}_i}{\partial x_j} - \tau_{ij}\right] + S_i \tag{2}$$

$$\frac{\partial}{\partial x_i}(\rho_g \bar{u}_i T) = \frac{\partial}{\partial x_j}\left(\frac{k + k_t}{c_p}\frac{\partial T}{\partial x_j}\right) + S_T \tag{3}$$

$$\frac{\partial}{\partial x_i}(\rho \bar{u}_i c_s) = \frac{\partial}{\partial x_j}\left(D_s \rho \frac{\partial c_s}{\partial x_j}\right) + S_s \tag{4}$$

$\tau_{ij} = \rho_g \overline{u_i' u_j'}$ is the Reynolds stress tensor which related to the average velocity gradient and turbulent viscosity of the flow. Where ρ_g is the gas density; $\bar{p}$ is the mean pressure; $\bar{u}_i$ and $\overline{u_i'}$ are the gas mean velocity and the gas mean fluctuating velocity, respectively ($i, j = 1, 2, 3$); T is the temperature; S_i, S_T and S_s are the source terms of momentum, energy and species, respectively; k and k_t are the molecular and turbulent thermal conductivity, respectively; c_p is the specific heat capacity; c_s is the volume concentration of component s; D_s is the diffusion coefficient of component s.

2.2. Discrete phase

Once the gas flow field is known, particle trajectory can be computed. In this study, the volume ratio of liquid-phase is less than 10%. So the liquid-phase is treated as discrete phase in the Lagrangian frame by defining the injection type, velocity, diameter and so forth (Li et al., 2008). The particle trajectory is calculated based on force balance by using the local continuous phase conditions as the particle moves along with the gas flow. These forces include the drag force, gravity and Saffman (Li et al., 2003). But the buoyancy, virtual mass and Basset term force are neglected because of the small ratio of fluid-to-particle density (Li et al., 2008; You et al., 2002). The particle–particle interaction and the effects of particle on the gas flow are also negligible due to the formulation assume that dispersed phase is sufficiently dilute. These treatments have been widely accepted for the dilute flow simulations (Buwa et al., 2006; Marocco and Inzoli, 2009; Narasimha et al., 2005). Then the momentum equation for a particle in the gas–liquid two-phase flow can be expressed as

$$\frac{du_p}{dt} = F(\bar{u} + u' - u_p) + g\frac{\rho_p - \rho_g}{\rho_p} + F_X \tag{5}$$

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