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Number Simulation of Heterogeneous Condensation of Water Vapor on Fine Particles in Growth Tube by Population Balance Model

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The emission of fine particles produced in coal combustion had been causing serious environmental and health problems. The heterogeneous condensation of water vapor on fine particles as a preconditioning technique for the removal of fine particles from flue gas is very promising in the future which has been proved by many works. This investigation adopted the k-epsilon turbulence model coupled with the population balance model（PBM）to simulate the performance of heterogeneous condensation of water vapor on fine particles in a growth tube. The supersaturation vapor environment can be achieved by adding water vapor in the inlet of the growth tube. The simulation results show that the particle growth is related to the distribution of the supersaturation in the growth tube. When the supersaturation is not enough, the particles stop growing. This agrees with the experiments that has been implemented previously. The effect of gas velocity and the concentration of the fine particles were analysed as well. The flue gas velocity decreasing will lead to the increasing of flue gas residence time in the growth tube. The high residence time is favourable for particle growth. As the initial particle concentration increases, the effect of particle growth is more obvious under the given supersaturation environment.

1. Introduction

Atmospheric inhalable fine particles PM2.5 are the primary pollutant in urban air, and have an important impact on the living environment. Vairo et al. (2014) used dispersion modelling to simulate the atmospheric emissions from a fossil fuel power station. Mancuso et al. (2014) analysed the factors of environment and safety in a power plant. The fine particles PM 2.5 are mainly produced in coal combustion in coal-fired power plant. PM 2.5 refers to the particle aerodynamic equivalent diameter less than $2.5 \cdot 10^{-6}$ m. The emissions of fine particles caused serious pollution in the environment and it is harmful to human health (Kim, 2015). At present, one of the important methods for removing fine particles is to make fine particles grow into larger particles, which could be removed by electrostatic precipitator. Droplets growth by heterogeneous condensation of water vapor as a preconditioning technique for removal of the fine particles from flue gas was investigated experimentally in a wet flue gas desulfurization (WFGD) system using spray scrubber as scrubber. The removal efficiency of the fine particles decreases with increasing of the initial particle concentration (Bao, 2013). Hao et al. (2016) proposed a novel process for fine particles abatement via heterogeneous vapor condensation coupling two impinging steams (TIS) technique. The results indicated that the removal performance of fine particles by this process was influenced by flue gas velocity of opposing jets in TISCGC (Two impinging steams condensational growth chamber), additive amount of steam or humid air and the desulfurized flue gas temperature. Porstendorfer et al. (1985) investigated the heterogeneous condensation of vapor on Ag and NaCl particles and observed the significant dependence of the heterogeneous condensation on particle size and surface properties. Chen et al. (1998) investigated the heterogeneous nucleation of water vapor on monodisperse submicrometer particles in a flow cloud chamber. It is concluded that the macroscopic theory of heterogeneous nucleation leads to significant underestimation of the nucleation rate and prediction of higher critical supersaturation than that experimentally measured. Xu et al. (2017) studied the heterogeneous condensation of water vapor on particles at high concentration. The

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residence time is in favour of the particle enlargement which depends on the supersaturation level. Additionally, the residence time extension would weaken the vapor depletion on particle enlargement caused by particle number increasing. Tammaro et al. (2012) investigated the heterogeneous condensation of submicron particles in a growth tube. The particles produced by a model ethylene/airflame by heterogeneous condensation of water vapor. The big difference between condensation steam and liquid temperature is in favour of the particle enlargement. Yu et al. (2013) simulated the water vapor condensation on an insoluble spherical particle by population balance model. When the supersaturation increases, the particle growth is obvious.

In this paper, the changes in the parameters of heterogeneous nucleation process which did not investigated in the previously experiments is described in details，such as the distribution of supersaturation and the distribution of particle as shown in the Figure 3(a) and Figure4. This simulation enriched heterogeneous nucleation theory and had practical application value.

2. Model

For the study of gas-solid two-phase flow, the Euler-Euler two-fluid model is the main method of simulation. We adopted the k-epsilon turbulence model coupled with the population balance model（PBM）to simulate the performance of heterogeneous condensation of water vapor on fine particles in the growth tube based on the Euler-Euler two-fluid model. The particle is regarded as continuous.

2.1 Heterogeneous Nucleation Process

There are many studies on the mechanism of fine particles growth in supersaturated water vapor field. It is considered that the water vapor condensed on the surface of the fine particles is the main mechanism of fine particle growth. According to the classical heterogeneous condensation theory of Fletcher (Fletcher et al., 1958), the water vapor condenses spontaneously on the surface of the particles when the supersaturation exceeded the critical supersaturation. The supersaturation environment was achieved by adding humid vapor in the inlet of the growth tube. The influence of different environmental parameters on the heterogeneous nucleation process of water vapor is reflected by the growth of particles in the growth tube.

2.2 Population Balance Model

In the research of the gas-solid two-phase flow, population balance model can describe the particle size changes in multiphase flow. These changes are caused by some physical phenomena, such as nucleation, growth, aggregation and breakage etc. The particle equilibrium equation is as follows:

$$\frac{\partial}{\partial t}\left[n\left(V,t\right)\right]=B_{ag,i}-D_{ag,i}=\frac{1}{2}\int_{0}^{V}a\left(V-V'\right)n\left(V-V'\right)n\left(V',t\right)dV'-\int_{0}^{\infty}a\left(V,V'\right)n\left(V,t\right)n\left(V',t\right)dV' \tag{1}$$

where $B_{ag,i}$ denotes particle generator, $D_{ag,i}$ denotes particle extinction, value 1/2 ensures that the same agglomeration process will not be counted two times). There are three methods can be used to solve the problems, the partition method, the moment method and the Monte Carlo method. In this paper, we choose the partition method, because its calculation precision is high. It can be seen that the changes of the particle size in the simulation results by population balance model. The effects of particle aggregation and particle breakage are ignored. The kernel function of the growth process refers to the particle growth equation of Xiong (2011):

$$I=\frac{dm_p}{d\tau}=\frac{4\pi r_p(S-1)}{\frac{L_v}{K_aT_\infty}(\frac{L_vM_v}{RT_\infty}-1)+\frac{RT_\infty}{D_vM_vp_s(T_\infty)}}f(Kn) \tag{2}$$

$$f(Kn)=\frac{1+Kn}{1+1.7Kn+1.333Kn^2} \tag{3}$$

$$Kn=\frac{l_v}{r_p} \tag{4}$$

where I denotes water vapor flux, $kg\cdot s^{-1}$; m_p is condensate droplet quality, kg; τ denotes t, s; r_p denotes droplet radius, m; and S is super saturation, which can be calculated as follows:

$$S=\rho_{v,\infty}/\rho_s(T_\infty) \tag{5}$$

where $\rho_{v,\infty}$ and $P_{v,\infty}$denotes the environmental water vapor density and pressure respectively); ρ_s and P_s denotes the surface balance of water vapor density and pressure of droplets, L_V is phase change latent heat, J·kg^{-1}, M_V denotes moisture mass of water vapor, kg·mol^{-1}; T_∞ is the temperature of environment, K; R=8.31J·mol^{-1}K^{-1}, and K_α denotes air thermal conductivity, W·m^{-1}·K^{-1}, which can be obtained:

$$K_a = 10^{-3}(4.39 + 0.071T_\infty) \tag{6}$$

where D_V is the water vapor diffusion coefficient in air, m^2·s^{-1};

$$D_v = 0.211 \times 10^{-4} \frac{p_0}{p}(\frac{T_\infty}{T_0})^{1.94} \tag{7}$$

2.3 Physical Model

In this paper, we use a growth tube model with an internal diameter of 1.5 cm and a length of 40 cm. The effects of gravity is ignored. The boundary condition of the inlet is velocity inlet. The boundary condition of the inlet is outflow. The density of SiC(silicon-carbide) is 3,170 kg/m^3. The simulation use monodisperse particles. The growth tube is a part of the phase change chamber which is used in the wet desulfurization system to remove the fine particles experiment by heterogeneous nucleation to reflect the change of the parameter details. It can be designed appropriately in different practical application. The simulation is a deep study of the previous experiments, so the simulation results need not experiment verification.

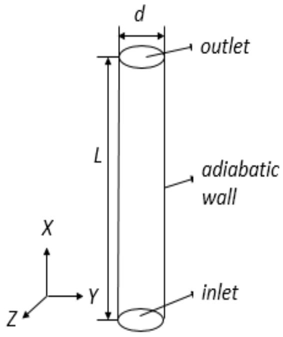

Figure 1: Growth tube model

3. Results and discussion

3.1 Supersaturation

The profiles of supersaturation in the axis of growth tube are described by employing a heat and mass transfer modelling. It can be seen in Figure 2 that the supersaturation in the growth tube decreases with the flue gas temperature increases. The supersaturation decreases along the growth tube height at the same temperature.

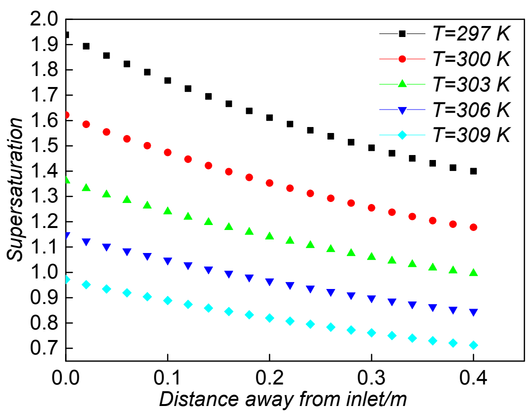

Figure 2: The profile of supersaturation in the axis of growth tube

Figures 3(a) and 3(b) show that the supersaturation and temperature distribution in different sections along the growth tube axis. The farther away from the inlet, the smaller the saturation. The temperature gradually increases with the distance away from the inlet increases. The reason is that the heterogeneous nucleation process consumed supersaturation and the latent heat was released when the water vapor is condensed on the surface of particle. The distance between each curve becomes small with the distance away from the inlet. It is indicated that the supersaturation is high at the inlet and the water vapor condensation rate is fast which lead to the temperature rises quickly. The reaction rate decreases and the temperature raises slowly with the supersaturation decreases.

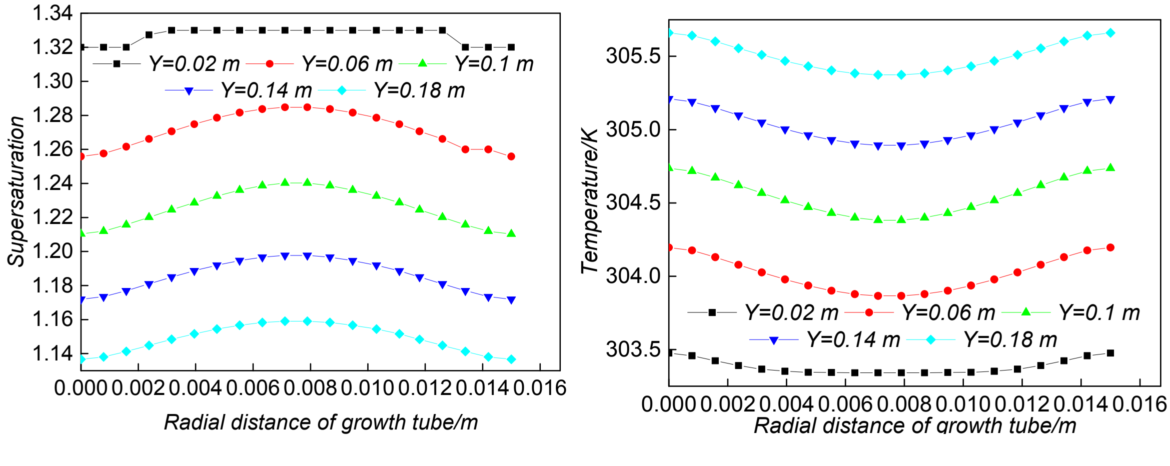

Figure 3: (a) The supersaturation distribution in different sections (b) The temperature distribution in different sections

The distribution of different size particles along the growth tube axis is described in Figure 4. The temperature is 303 K and the supersaturation of inlet is 1.36. The particle size increases along the growth tube height. The large particles are concentrated in the outlet. Firstly, $0.1 \cdot 10^{-6}$ m particles enter the growth tube and contact with the water vapor. The particles grow into $0.137 \cdot 10^{-6}$ m under the enough supersaturation environments. And then the $0.137 \cdot 10^{-6}$ m particles flow with gas and grow to larger particles. Due to the supersaturation decreases along the growth tube height in Figure 1, the particles grow into $2.04 \cdot 10^{-6}$ m and the corresponding location is 0.3 m and the particles stop growing until flowing to the outlet. The reason is that the supersaturation decreases along the growth tube height, the saturation of the location at 0.3 - 0.4 m cannot sustain the particle growing.

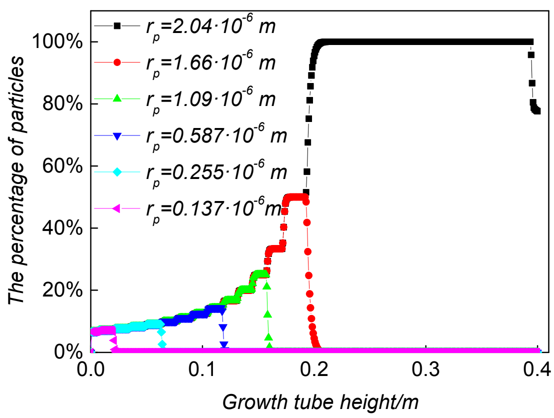

Figure 4: The particle distribution in the axis

3.2 Flue Gas Velocity

Figure 5 gives the results of flue gas velocity effect on fine particles enlargement. The supersaturation of inlet is 1.36. Particle volume fraction is 0.0005 and the temperature of flue gas is 303 K. With the decreasing of the flue gas velocity, the number density (denotes the number of particles per unit volume) of particle decreases in the range of 0.1 to $0.89 \cdot 10^{-6}$ m, as the peak value declined in Figure 5. However, the number density of particle increases in the range of 1.6 to $2.04 \cdot 10^{-6}$ m. The decreasing of flue gas velocity will lead to the increasing of flue gas residence time in the growth tube. The fine particles of the flue gas could contact with the vapor fully. It can be explained as follows, the residence time extension leads to more vapor transfer onto the particles under enough supersaturation for the same quantity particles. The high residence time is favourable to particle growth. Then, small-size particles grow into bigger particles. The high flue gas velocity reduces the residence time of particles in the growth tube. Water vapor condenses on the surface of particles decreases. Therefore, the number density of big particles is much less compared with that of low flue gas velocity. It can be found that the low flue gas velocity leads to high residence time and promotes the particle enlargement.

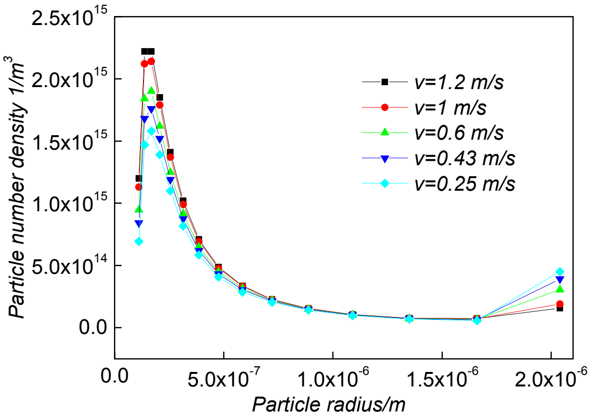

Figure 5: Flow gas velocity effect on fine particles enlargement

3.3 Volume Fraction

Figure 6(a) shows the initial particle volume fraction effect on fine particles enlargement. The temperature of flue gas is 303 K, the supersaturation of inlet is 1.36 and the flue gas velocity is 0.43 m/s. When the volume fraction increases, the initial particle number increases. Under the same supersaturation environment, more particles grow up. More particles enlargements cause more water vapor condenses on the surface of particle, so the supersaturation of the outlet decreased with an increase of the initial particle number as shown in Figure 6(b). When the flue gas enteres the growth tube, the particles enlarge from $0.1\cdot$to $2.04\cdot10^{-6}$ m. Firstly, the supersaturation environment can afford a large quantity particles grow into the range of $0.1\cdot10^{-6}$ m to $1.5\cdot10^{-6}$ m. But with more water vapor condensed, the supersaturation decreases and cannot sustain all particles grow into $2.04\cdot10^{-6}$ m. So the number density of $2.04\cdot10^{-6}$ m particle increases slowly.

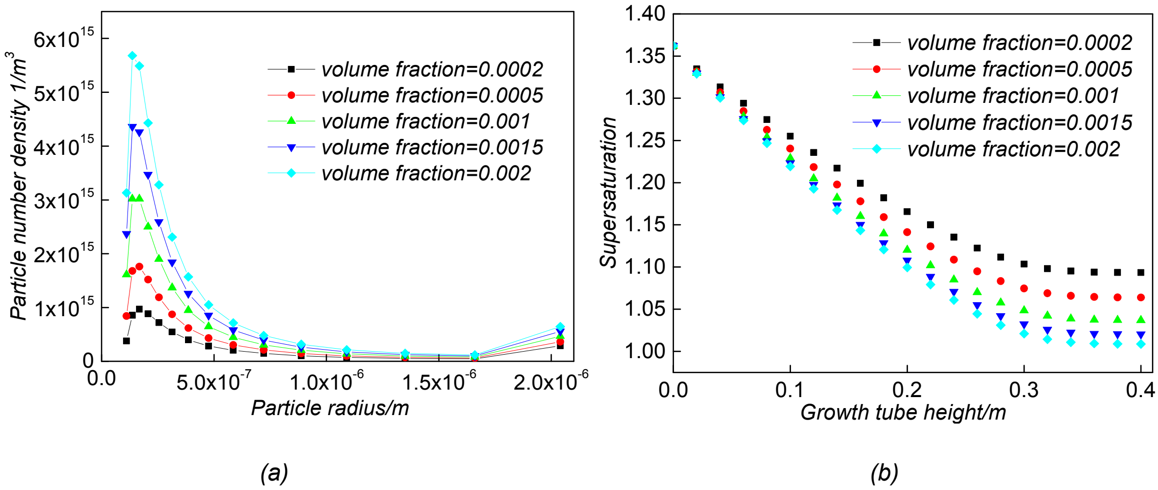

Figure 6: (a) Volume fraction effect on fine particles enlargement (b) Supersaturation distribution in the growth tube

4. Conclusions

(1) By adding humid vapor in the inlet of the growth tube, supersaturation environment can be obtained. The supersaturation in the growth tube decreases with the flue gas temperature increases. When the

supersaturation is high, the heterogeneous nucleation rate is high and the temperature of the tube rises sharply. The particle size increases along with the growth tube axis.
(2) Flue gas velocity is an important industrial operating parameter. The low flue gas velocity is favorable to particle growth. So, the number of large particles is high.
(3) There are more water vapor condenses on the surface of particle with the particle volume fraction increases. The supersaturation in the outlet decreases and the number density of large particles increases under the same initial supersaturation.
(4) The distribution of supersaturation and temperature in the growth tube can fully reflect the change of environmental parameters during the removal of fine particle by heterogeneous nucleation. It has a certain reference value to improve the efficiency of removal of fine particles. The industrial growth tube of the heterogeneous nucleation process can be designed according to the boundary conditions of this growth tube model.

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