Agglomeration Modelling of Sub-Micron Particle during Coal Combustion Based on the Flocculation Theory

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Abstract: The monte carlo method was used to simulate chemical agglomeration of sub-micron particle which based on the flocculation model of the water processing, the influence of different agglomeration solution volume on sub-micron particle agglomeration was investigated. Simulation results show that the growth of particle mean diameter and the decrease of particle number are fast at the initial stage of agglomeration, and the speed of them increase with agglomeration solution volume increasing. After achieving stability, as a whole, the particle mean diameter is almost in proportion to agglomeration solution volume. At the last stage of agglomeration, particle number follows a similar bimodal distribution, which is varying with different agglomeration solution volumes. When agglomeration solution volume is 2 ml/min, the peak value of diameter is the biggest.

Keywords: chemical agglomeration，sub-micron particle，flocculation，simulation

1 INTRODUCTION

Existing dust collecting equipments in coal-fired power plant have less efficient removal of sub-micron particle (PM2.5). A large number of sub-micron particles are emitted into the atmosphere, causing severe environmental pollution[5]. Sub-micron particles grow up because of chemical agglomeration, and are removed at last by ESP, which opens up a novel method to control sub-micron particles emission. Foreign scholars simulate agglomeration phenomenon by the experiential formulas which come out from experiments. For example, soot agglomeration in a Microgravity Diffusion Flame has been study by Ezekoye[4], and experiential formulas is utilized to forecast the diameter and concentration of soot aggregate. Yakup Cebeci[2] has study the experimental data statistics of particles agglomeration in flue gas, and gets the experience formula of particle aggregate size distribution. Thanks to the limit of empirical formula, it can not be used in further study on agglomeration process and micro-mechanism of agglomeration. In this paper, the newest Flocculation model in water treatment is choosed and modified a little, so that it applies to the simulation of chemical agglomeration. Monte Carlo algorithm is used to be focused on particle dynamic evolution during particle agglomeration process.

2 MODEL

The most fundamental difference between chemical flocculation agglomeration and ordinary spontaneous agglomeration is that it take palce the initiative adsorption between solid particles and liquid droplets, thereby greatly increasing the agglomeration rate of particles. There exist two mechanisms about the agglomeration between them: (a) When the diameter of particles is similar to the diameter of droplets, the initiative absorption will take place, droplets form a liquid film on the surface of particles, and then the particles agglomerate with each other, causing the occurrence of flocculation, which will greatly promote the efficiency of agglomeration between the particles. The main reason is the agglomeration molecule in the liquid film improve the efficiency of agglomeration through all kinds of flocculation mechanisms: the double-layer compression, charge neutralization, and bridging action. Fig. 1 shows the agglomeration liquid film mechanism. (b) When the droplets is much larger than the particles, after contious adsorption, droplet surface will be embedded by many solid particles, finally formatting the flocculation which is similar to the flocculation of the first agglomeration mechanism. Fig. 2 shows the Immersion agglomeration mechanism.

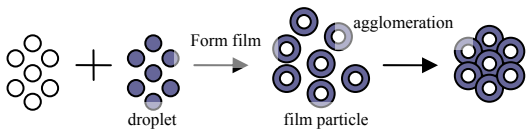


Fig. 1 Distribution agglomeration mechanism

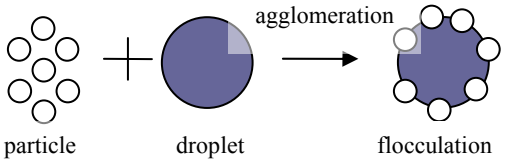


Fig. 2 Immersion agglomeration mechanism

No matter which kind of mechanism, the first formation is all the primary flocculation, which is just the liquid film particle, inner is particles and surface is liquid film. This occurred constantly over the two mechanisms to form the secondary flocculation, and three-level flocculation (Fig. 3).

The particles chemical agglomeration process depends

primarily on agglomeration mechanism, kernel functions. Under the six assumptions, Smoluchowski[8] establishes the corresponding flocculation kernel functions. But for chemical agglomeration, these assumptions have large difference with actual situation, so I have modified them: (a) All the particles adsorb each other actively to be agglomerated finally, not by rigid collision. then the agglomeration efficiency is much higher, in general 0.8–0.9; (b) Fluid motion undergoes turbulent shear; (d) after the formation of flocculation, it also could occur the breakage of it, but we overlooked its impact and consider the particles agglomeration emphatically; (e) Before and after adsorption all particles is not the solid sphere, but inner is the solid core and outer is the expansion layer with better wettability; (f) Absorption will take place between the particles, particles and droplets, the droplets; However, different types of adsorption own different agglomeration kernel function, the related parameters are set by the experimental data.

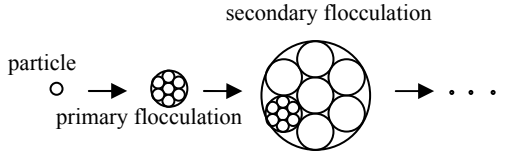


Fig. 3 Stepwise growth agglomeration flocculation

The Brown agglomeration always exists for the sub-micron particles, and in the chemical agglomeration process, agglomeration caused by fluid shear and the velocity gradient is also very clear. Particle flocculation kernel functions are improved, including Brownian coagulation kernel, turbulent shear kernel and different sedimentation kernel:

Brownian coagulation kernel[3]:

$$\beta_{Br} = (\frac{2kT}{3\mu_g})(\frac{1}{d_i} + \frac{1}{d_j})(C_i d_i + C_j d_j) \tag{1}$$

Turbulent shear kernel[9]:

$$\beta_{Sh} = \sqrt{\frac{8\pi}{15}}(G)^{\frac{1}{2}}(d_i + d_j)^3 \tag{2}$$

Different sedimentation kernel[7]:

$$\beta_{DS} = (\frac{\pi g}{72\mu_g})(\rho_p - \rho_g)(\eta_i d_i + \eta_j d_j)^3 \,|\, \eta_i d_i - \eta_j d_j \,| \tag{3}$$

Overall agglomeration kernel:

$$\beta = \beta_{Br} + \beta_{Sh} + \beta_{DS} \tag{4}$$

where, k is the Boltzmann constant(1.138054×10^{-23}), T is the environmental absolute temperature. The agglomeration is simulated in the flue environment before electrostatic precipitator, so the environmental absolute temperature T=423 K, the density of flue gas ρ_g=1.193 kg·m^{-3}, the viscosity of flue gas μ_g=1.83245×10^{-5} kg·m^{-1}·s^{-1}, the density of agglomeration agent ρ_w=997.45 kg·m^{-3}, the viscosity of droplets μ_w=9.591×10^{-4}kg·m^{-1}·s^{-1} , the density of particles ρ_p= 2270 kg·m^{-3}.

$$C = 1 + K_n\left[a_1 + a_2 \exp(-a_3 / K_n)\right] \tag{5}$$

where, C is the Cunningham slip factors of particles and droplets , the dimensionless constants a_1, a_2 and a_3 are taken as 1.142, 0.558 and 0.999 respectively, following Allen and Raabe (1985)[1]; K_n is the Knudsen number.

G is the velocity gradient in the flue gas turbulence field, $G = \varepsilon / \upsilon$. ε is the mean energy dissipation rate in the flue gas turbulence, $\varepsilon \approx 25 \mathrm{ergg^{-1}\,s^{-1}}$, υ is the kinematics viscosity of flue gas (3.49×10^{-5} m^2/s)[9]. d_i and d_j is the diameter of particle or drolet, but in the simulation calculation, flocculation diameter is used, ηd_i. As long as the distance between the particles is smaller than the sum of ηd_i and ηd_j, the flocculation agglomeration will take place. η is the coefficient of flocculation diameter, mainly related to the viscosity of agglomeration agent, the agglomeration film thickness, the difference between the density of particles and droplets, the relative velocity between particles, particle and droplet.

$$\eta = k(\frac{\mathrm{d}\, v \Delta\rho}{\mu})^a \tag{6}$$

where, k is the agglomeration coefficient, and set by the experimental data, in general 1.2–1.5; μ is the viscosity of agglomeration agent, d is the agglomeration film thickness, if particle, just the 10% diameter of particle; if droplet , just the diameter of droplet , v is the absolute value of the relative velocity between particles, particle and droplet, $\Delta\rho$ is the difference between the density of particles and droplets, if doplet, just the density of droplet. a is a dimensionless index, in general 1.15–2.15.

3 ALGORITHM

In this paper, the Monte Carlo algorithm is used, and any circumstances of all particles which may occur are considered at a right time step, and they are mutually independent. In the algorithm each simulated particle is on behalf of a certain number of real particles in actual system, each simulated particle owns a certain number-right-value. The number-right-values of all the simulated particles change with time. In the algorithm the weighted virtual particles, a group of the same or similar scale of the actual particles which have the same attributes and behavior, are representatives of one or several virtual particles which owns the appropriate number-right-value[6]. In the calculation region V (in the simulation, V = 1 m^3), the actual number of particles, N, the number of virtual particles, N_f, the times of agglomeration for virtual particle i in unit time:

$$C_i = \frac{1}{V^2}\sum_{j=1, i\neq j}^{N_f}(\beta_{ij} \times w_j) \tag{7}$$

where, w_j is the number-right-value of virtual particles j, β_{ij} is the agglomeration kernel of virtual particles i and j. And the time of virtual particles i agglomeration for once is t_i=1/C_i. The time step Δt must be less than or equal to the minimum of agglomeration time scale[6].

4 NUMERICAL SIMULATION

4.1 Initial Conditions

The dust produced by the coal-fired boilers before ESP follows three modes distribution, the sub-micron dust region of 0.1 μm as the center, the minor-meter dust region of 2.0 μm as the center and the AMD-meter dust region of 5.0 μm as the center[6]. This paper is the focus of the study to agglomeration flocculation process in the minor-meter region of 2.0 μm as the center. I suppose the initial distribution of the simulated particles and droplets meet lognormal distribution. The lognormal distribution is:

$$n(d)=\frac{N}{\sqrt{2\pi}\ln\sigma}\exp[-\frac{\ln^2(d/d_m)}{2\ln^2\sigma}]\frac{1}{d} \quad (8)$$

where, N, d_m and σ are the total number of dust particle or droplet, the geometrical mean diameter and the geometric standard deviation. Initial enactment: d_{pm}=2.5μm, N_p = 1×10^{10}/m^3, σ_p = 1.35. In simulation the volume of flue gas V=1 m^3, the diameter range of particle is $\ln d_{pm}-3\ln\sigma_p \le \ln d_p \le \ln d_{pm}+3\ln\sigma_p$, just 1.0161 μm–6.1509 μm. The diameter of particle will be divided into 100 range, set up the total number of virtual particles, 4000.

Simultaneously, the diameter range of droplet is $\ln d_{wm}-\ln\sigma_w \le \ln d_w \le \ln d_{wm}+\ln\sigma_w$, just 12.5 μm–50.0 μm. The diameter of droplet will be divided into 100 range, set up the total number of droplet, 2000. The other parameters of droplet are as follows Table 1.

Table 1 Agglomeration droplet parameter

Volume of agglomeration agent v/ (ml·min^{-1}·m^{-3})	Number of droplet N_w/m^{-3}	Geometrical mean diameter of droplet d_{wm}/mm	Geometric standard deviation of droplet σ_w
1	1.23×10^7	25	1.5
2	2.46×10^7	25	1.5
5	6.15×10^7	25	1.5

4.2 Evolution Process of Particles

Seen from Fig. 4, in the early 100 s around of agglomeration, the mean diameter of particle increase rapidly with time. The greater flow of agglomeration, growth rate is faster. Without agglomeration agent the mean diameter is the smallest. However, when the flow is 1 ml/min, in the latter part of the agglomeration, the mean diameter of particles still maintain a certain growth rate, and surpasses the mean diameter when the flow is different. So the flow can not be too large or too small, because the smallest number of droplets will also affect the absorption between the particles and droplets. In the Fig. 5, after the accession of agglomeration agent, the number of particles decreased faster significantly. Also in the early 100 s of agglomeration, the number of particles decreases faster, and the greater flow and the faster underspeed; when the flow is 1 ml/min or 2 ml/min, the number of particles still has a decreasing trend. This shows that 1 ml/min and 2 ml/min are the best flow.

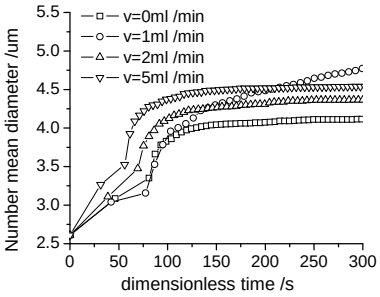


Fig. 4 The evolution of particle mean diameter

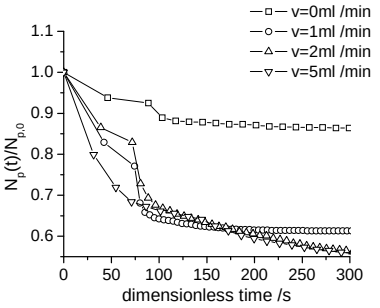
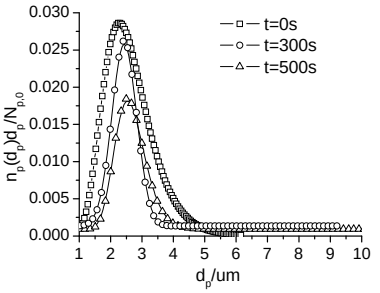
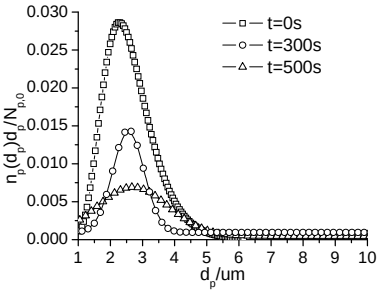


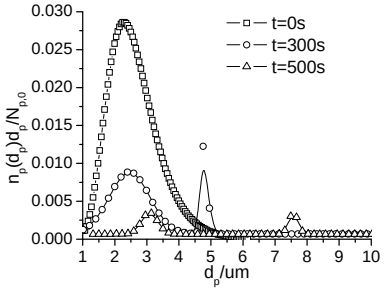
Fig. 5 The evolution of particle number



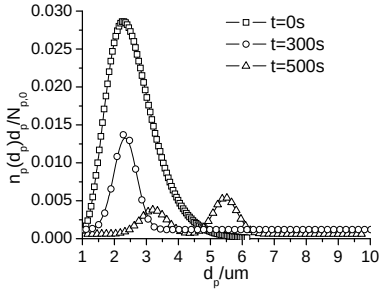
(a) v = 0 ml/min



(b) v = 1 ml/min



(c) v = 2 ml/min



(d) v = 5 ml/min

Fig. 6 The evolution of particle size distribution when different agglomeration agent volume

Seen from Fig. 6(a), with the passage of agglomeration time, the number of particles decreases to a certain extent, but the degree is low, the diameter of particle also increase slightly. And in the Fig. 6(b) when the flow of agglomeration agent is 1 ml/min, the number of particles decreases to a greater extent, and after 500s, the peak value of particles number has dropped to around 0.005, the agglomeration effect is remarkable.

In the Fig. 6(c) when the flow of agglomeration is 2 ml/min, the number of particles decreased at a faster pace, after 300s the peak value of particle number decreases to 0.008. And a sub-peak has been formed in the right side 5 μm of the main peak, after agglomeration of the small particles, the formed large particles mainly concentrate at 5 μm in diameter, the peak is about 0.008. After 500 s, the main peak of particles number moves to the right 3 μm, the peak value has also been further reduced to 0.004.

In Fig. 6(d) comparing the flow of agglomeration agent 5 ml/min to 2 ml/min, the number of particles decreases at a slowed pace, increasing trend of particle diameter is not as remarkable as the trend of 2 ml/min. After 200s only a peak of particles number at 2.5 μm exists, the peak value is probably around 0.015. after 500 s, the number of particles follow a bimodal distribution, the main peak is at 3 μm with the value of 0.005, the sub-peak is at 5.5 μm with the value of 0.006. To sum up, when the flow is 5 ml/min, the effect of agglomeration is not good as the 2 ml/min, but this would consume more agglomeration agent, not economic. So the bigger flow is not always better.

5 CONCLUSIONS

In the early 100 s of agglomeration, the mean diameter and number of particle increase rapidly at a larger pace. The greater flow of agglomeration, growth rate is faster. After achieving stability, the overall trend is that the greater flow of

agglomeration, the greater diameter. Without agglomeration agent the mean diameter is the smallest, and the number of particles is the largest. After the addition of agglomeration agent, the peak value at 2.5 μm decreases to a larger extent, but the latter part of agglomeration the number of particles follows a bimodal distribution. When the flow is 2 ml/min, the effect is the best.

ACKNOWLEDGEMENTS

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