Numerical Simulation Research on Agglomeration between Coal-fired Fly Ash Fine Particulate and Atomized Droplets

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Abstract. In this paper, the interaction process between atomized droplets and particles after spraying chemical agglomeration solution was numerically simulated, the force model of particles in agglomeration solution was established, and the effects of density, viscosity, flow rate of agglomeration solution, and diameter of atomized droplets and other factors on the velocity, quality, diameter and number of particles after agglomeration were analyzed. The simulation results showed that the speed, mass, diameter and number of particles after agglomeration were greatly affected by the physical and chemical parameters of the chemical agglomeration solution. Increasing the density and viscosity of the solution could increase the variation trend of each characteristic quantity of particles. As the flow rate of agglomeration solution and diameter of atomized droplets became larger, the collision probability between the solution and particles got higher as a result. Since the particles gradually agglomerated, their mass and diameter increased. As their speed gradually decreased, the probability of collision and agglomeration with chemical agglomeration solution decreased as well.

1. Introduction
China ranks first in the world in annual coal production and consumption. Fine particulate matter (PM2.5) emitted from coal combustion can enter the lungs due to its small particle size, causing various respiratory diseases and even lung cancer[1]. Existing dust removal technologies, including electrostatic dust removal and bag dust removal technologies, have a removal efficiency of 99.9% for coarse particles, but a lower removal efficiency for fine particles. A large number of fine particles cannot be captured and removed by dust collectors due to their small sizes[2]. In view of this situation, chemical agglomeration technology[3] was adopted. A spray gun was installed in the flue in front of the dust collector to inject chemical agglomeration agent into the flue through compressed air and fully mixed with flue gas. Under the action of agglomeration solution, fine particles were agglomerated into particles with larger size, and then captured by dust removal equipment.

Agglomeration phenomenon among particles has always been the focus of research in colloid science, materials science, physics and microbiology. Exploring the mechanism of particle collision agglomeration has always been the goal pursued by most scientific researchers. By clarifying the mechanism of particle agglomeration, we can better master the chemical agglomeration technology, thus applying it to the engineering and technical fields of air pollution control, sewage treatment, etc.

In the process of studying the agglomeration mechanism of fine particles, researchers have established various particle agglomeration models according to their own experimental research needs. Research by Schaefer and Mathiesen[4]shows that, according to the size and viscosity of agglomerated
agent droplets, the agglomeration mechanism can be divided into two types, namely distribution mode and immersion mode, as shown in Fig. 1. When the droplet size of the agglomeration solution was smaller than the particle size, or the two sizes were similar, it was mainly the distribution mode. In this mode, the droplets of agglomeration solution were uniformly wrapped on the surface of the particles, and then the droplets and the droplets were agglomerated together under the action of a liquid bridge to form agglomerates. When the droplet size of agglomeration solution was much larger than the particle size, it was mainly in immersion mode. In this mode, the particles adhered to the surface of the agglomeration solution droplets. Generally speaking, in the process of agglomeration, both modes existed. When the size of agglomeration agent drops was small, the viscosity was low and the speed was slow, the distribution mode dominated. When the size of agglomeration agent drops was large, the viscosity was high and the speed was fast, the immersion mode dominated. Goldszal and Bousquet[5] summarized the four stages of the combination of atomized droplets and particles according to the addition or moisture content of the solution when the agglomeration solution interacted with the particulate matter, as shown in Fig. 2.

Figure 1. Mechanism of distribution agglomeration and immersion agglomeration

Figure 2. State diagram of droplet and particle agglomeration process

2. Theoretical analysis of spray process of chemical agglomeration solutions

2.1. Collision model of agglomeration solutions atomized droplets with particles
A collision model between spraying droplets and particles was established. The effects of various factors on the agglomeration effect of particles after the agglomeration solutions were sprayed were simulated. After spraying the chemical agglomeration solution, atomized liquid drops were formed. They then collided with the fly ash fine particles and combined together to form larger particles[6, 7]. The model assumed the following:

- The particle size was characterized by the average particle size of fine particles of coal-fired fly ash and atomized droplets of chemical agglomerating agent;
- Assuming that the fly ash particles were agglomerated together after colliding and no longer separated. The shape of atomized droplets and particles before and after the agglomeration process were all regular spheres.
- Assuming that the fly ash particles had uniform distribution of particle mass and density. The total mass and volume of the system including atomized droplets and particles were conserved before and after agglomeration;
- Assuming that the particles were continuously dynamic during the air flow process. The movement of gas molecule was ignored.
- Assuming that tension of the agglomeration solution remained unchanged.

2.2. Force analysis of particles in solutions

After the fly ash particles were dissolved in the agglomeration solution, colloidal suspension was formed. In solution, the particles were affected by various forces. According to the force type classification, including volume force, such as gravity and electrostatic force; area force, including buoyancy and drag force. The trajectory and heat transfer of particles in solution were calculated by various equilibrium forces acting on particles by droplets and heat transfer caused by convection/radiation, respectively[8]. In Cartesian coordinate system, the force balance equation of particles in the X-axis direction was:

$$\frac{dv_p}{dt} = F_D(v_l - v_p) + \frac{6\pi\eta v_p (\rho_p - \rho)_p}{\rho_p} + F_x$$

Among them, $F_D(v_l - v_p)$ was the drag force, $F_b$ was the additional force, including thermophoretic force $F_b$, brownian force $F_b$, Saffman lift $F_b$, Van der Waals force $F_v$, electrostatic force $F_e$, liquid bridge force $F_b$ and Basset force. Besides, the drag force was:

$$F_D = C_D \frac{\pi d_p^2 \rho (v_l - v_p)^2}{2}$$

$C_D$ was the drag coefficient, which was related to Re. $d_p$ was the particle diameter, $v_l$ was the atomized droplet velocity, $v_p$ was the droplets velocity, and Re was:

$$Re \equiv \frac{\rho d_p |v_p - v_l|}{\mu}$$

According to the research of Haider and Levenspiel[9], the drag coefficient $C_D$ was:

$$C_D = \frac{24}{Re} \left(1 + b_1 Re^{b_2}\right) + \frac{b_3 Re}{b_4 + Re}$$

3. Analysis of Factors Affecting Particle Aggregation Effect

During the time period of t to t+Δt, the volume increase of atomized droplets of agglomeration solution caused by adhering particles was expressed by the volume of particles contained in the volume swept by the droplets as follows:

$$\left(v_l - v_p\right) \frac{\pi}{4} d_p^2 n_0 \frac{\pi}{6} d_p^3 dt$$

According to droplet evaporation drying theory, the volume reduction due to evaporation can be expressed as:

$$\frac{2\pi d_p K (1 + 0.276 Re^{0.6} Sc^{0.33})}{\rho l Y} \Delta T_m dt$$
So, the formula of particle velocity change with time was:

\[
\frac{d v_a}{dt} = \frac{18 \mu (v_p - v_l)}{\rho d^2_a} - \frac{(v_l - v_p) 2 \eta d^2 n_0 m_p}{m_a + (v_l - v_p)^2 d^2 n_0 m_p} \tag{7}
\]

The formula for the change of particle mass \( m_a \) with time was

\[
\frac{d m_a}{dt} = \left[ (v_l - v_p) \frac{\pi}{4} d^2 n_0 m_p \right] - \frac{2 \eta d_k (1 + 0.276 Re^{0.5} Sc^{0.33}) \Delta T_m}{\gamma} \tag{8}
\]

The initial parameters of chemical agglomeration solution droplets and fly ash particles were set as follows:

| Table 1. Initial Parameters of Numerical Simulation of Chemical Agglomeration. |
|-----------------|--------|----------|
| Item            | Unit   | Value    |
| Smoke Temperature | K      | 423/373  |
| Initial Velocity of Particles | m·s\(^{-1}\) | 5        |
| Initial Diameter of Particles | µm     | 0.1      |
| Initial Mass of Particles | µg     | 0.001×10\(^{-3}\) |
| Initial Number of Particles | -      | 10000    |
| Particle Viscosity | kg·m\(^{-1}\)·s\(^{-1}\) | 2.4×10\(^{-5}\) |
| Initial Velocity of Agglomeration Solution Droplets | m·s\(^{-1}\) | 12       |
| Initial Diameter of Agglomeration Solution Droplets | µm     | 20/15/10 |
| Density of Agglomeration Solution Droplets | kg·m\(^{-3}\) | 2400/1800/1200 |
| Viscosity of Agglomeration Solution Droplets | mPa·s | 260/200/130 |

3.1. Effect of density of chemical agglomeration solution on agglomeration effect

This section simulated the effect of spraying three kinds of chemical agglomeration solutions with different densities on the characteristic quantities of particles after agglomeration. The solution densities were 2400 kg·m\(^{-3}\), 1800 kg·m\(^{-3}\) and 1200 kg·m\(^{-3}\), respectively.
As can be seen from Fig. 3, after the chemical agglomeration solution was injected, the speed of fly ash particles gradually decreased. When the time closed to 1s, the particle velocity tended to be stable. It showed that particles and droplets of the chemical agglomeration solution aggregated together to form polymers, and the speed reached a stable value. In addition, under the same conditions, the higher the density of the agglomeration solution, the faster the particle velocity decreased. In the same time, the particle mass increased faster after injecting the agglomeration solution with higher density. Aggregates formed by aggregation of agglomeration solutions and particles were easier to adsorb surrounding particles as their mass increased. Under the same conditions, the effect of spraying agglomeration solution with higher density was better. The diameter of the formed polymer was increased from 0.1 m to more than 0.6 m, and the effect was better than that of the agglomeration solution with lower density (0.5 m). After spraying chemical agglomeration solution, the particle number decreased significantly. Therefore, in order to improve the agglomeration efficiency, the density of agglomeration solution should be appropriately increased.

3.2. Effect of viscosity of chemical agglomeration solution on agglomeration effect
There were three kinds of chemical agglomeration solutions with different viscosities. The viscosities were 260 mPa·s, 200 mPa·s, and 130 mPa·s, respectively. The effect of the additive on the characteristic quantities of the agglomerated particles was investigated.
As shown in Fig. 4, solution with higher viscosity also have greater resistance to particles. Therefore, the particles were easier to be captured by the agglomeration solution with higher viscosity and the agglomeration efficiency was higher under the same conditions. Agglomeration solution with higher viscosity were easier to agglomerate with particles, thus increasing the mass of particles faster. Injecting agglomeration solution with higher viscosity increased the particle diameter more obviously. The initial particle size was 0.1 μm, the particle size increased to more than 0.7 μm 1 s later after the agglomeration solution with a viscosity of 260 mPa·s was injected. However, after the agglomeration solution with a viscosity of 130 mPa·s was injected, the particle size only increased to about 0.4 μm. Solution with higher viscosity had better capture effect on particles. Therefore, the particles were easier to aggregate and grew up, and the diameter change was more obvious. The initial particle number was about 10,000. After the agglomeration solution with a viscosity of 260 mPa·s was injected, the particle number decreased to about 4,000, which decreased about 60%.

3.3. Effect of flow rate of chemical agglomeration solution on agglomeration effect
The influence of spraying three kinds of chemical agglomeration solutions with different flow rates on each characteristic quantity after agglomeration was simulated. The flow rates were 0.05 kg·s⁻¹, 0.04 kg·s⁻¹, and 0.025 kg·s⁻¹.
Figure 5. Effect of flow rate of chemical agglomeration solution on characteristic quantity of particles after agglomeration

As can be seen from Fig. 5, the larger flow rate, the larger number of agglomeration solution droplets in the same time. As the mass was larger, the probability of collision between atomized droplets and particles was relatively increased. The diameter of particles increased faster when the agglomeration solution with larger flow rate was injected during the same time. As well as the diameter of agglomerates formed was larger. Therefore, in order to improve the agglomeration efficiency, the flow rate of agglomeration solution can be appropriately increased.

3.4. Effect of atomized droplet diameter on agglomeration effect

The influence of spraying three kinds of chemical agglomeration solutions with different diameters of atomized droplets on the characteristic quantities of particles after agglomeration was simulated. The droplet atomization sizes were 20 µm, 15 µm and 10 µm, respectively.

Figure 6. Effect of atomized droplet diameter on characteristic quantity of particles after agglomeration

As shown in Fig. 6, as the droplet diameter increased, the specific surface area of the droplet also increased. So was the collision probability between droplets and particles. Particles were easier to combine with droplets to form aggregates. Therefore, the particle speed drop faster. Under the same conditions, the mass and diameter of particles increased faster after spraying solution with larger atomized droplet diameter. Increasing the atomized droplet diameter could increase effective contact area with the particles. Therefore, properly increasing the atomized droplet diameter can effectively improve the agglomeration efficiency of fine particles.
4. Conclusions
In this paper, the interaction process between atomized droplets and particles after spraying chemical agglomeration solution was numerically simulated. The stress model of particulate matter in agglomeration solution was established. The effects of agglomeration solution density, viscosity, flow rate and atomized droplet diameter on velocity, mass, diameter and number of particles after agglomeration were analyzed. The main conclusions are:

The simulation results show that the speed, mass, diameter and number of particles after agglomeration were greatly affected by the physical and chemical parameters of the chemical agglomeration solution. Increasing density and viscosity of the chemical agglomeration solution properly can increase the variation trend of each characteristic quantity of the particles. Within a certain range, the larger the flow rate of agglomeration sloution and the larger the diameter of atomized droplets, the higher the collision probability with particles and the better the agglomeration effect.

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