

**Original Research Paper** 

# Numerical Analysis of Growth of Coal-fired Particles Promoted by Condensation of Water Vapour in Oversaturated Environment

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# ABSTRACT

A kinetics model was established to investigate the effects of condensation of water vapour on the growth of coal-fired particles. The effects of operating parameters on particle growth were numerically studied, including growth time, supersaturation, flue gas temperature and particle number concentration. The results showed that almost all the particles could grow rapidly more than 2.7 microns in tens of milliseconds. When initial super saturation is constant, the higher the temperature of flue gas, the larger the amount of condensable vapour and the final diameter of particles. Moreover, when the gas temperature is constant, the higher the degree of saturation, the larger the driving force for vapour condensation and the particle size distribution becomes narrower. Additionally, with the increasing of particle number concentration, the competition between particles for water vapour become more intense, and the final diameter for particles are smaller.

### INTRODUCTION

In recent years, frequent occurrence of haze weather has aroused people's extensive attention to fine particle matters. The particles with an aerodynamic diameter less than 2.5 microns are defined as  $PM_{2.5}$ . These small particles can not only cause serious environmental problems but also pose a serious threat to people's health (Curtis et al. 2006). As those fine particles commonly carry multiple hazardous and toxic substances, such as poisonous heavy metals, bacteria, viruses, acid oxides and so on. Even more seriously,  $PM_{2.5}$  could enter human respiratory tract and deposit in the lungs, and then participate in human blood circulation, which could induce a variety of diseases and causes serious harm to the functions of heart and lung (Bentayeb et al. 2012).

Analysis of the source of particulate matter in the ambient atmosphere shows that the flue gas emitted from the coal-fired power station carries a large amount of fly ash fine particles, which is one of the main sources of fine particles in the atmosphere (Hao et al. 2016a). At present, electrostatic precipitators are widely used in large coal-fired power stations to remove fly ash particles in the flue gas, and the mass removal efficiency can reach more than 99%. However, due to limited by the mechanism of charging, the removal efficiency of submicron particles is inefficient and a large number of fine particles are emitted into the atmosphere (Zhou et al. 2016). Therefore, it has become an urgent problem that how to remove fine particles more effectively. However, high removal efficiency could be achieved if the size of particle could be enlarged by means of preconditioning techniques such as heterogeneous condensation of water vapour (Tammaro et al. 2012), turbulent agglomeration (Chen et al. 2016), acoustic agglomeration (Liu et al. 2017) and chemical agglomeration (Hu et al. 2018) and so on.

According to many researchers, condensation of water vapour on the surface particles is one of the most promising preconditioning technologies to promote fine particle to be larger. Heidenreich et al. (1995) carried out the study of removing sub-micron quartz and paraffin oil particles in the tower by using the technology of multi-stage packed tower in series and alternately spraying cold and hot water. Yan et al. (2007) injected water vapour into the flue gas to achieve super saturation and coal-fired particles become larger by vapour condensation of steam in front of the scrubber, and the grown particles can be more effectively removed by wet scrubber. Fan et al. (2013) investigated the effects of different operational parameters on PM2 5 particle size distribution based on the theory of polydisperse particle. Wen et al. (2014) studied the condensation growth characteristics of soluble ammonium sulphate particles in supersaturated steam environment by numerical analysis. Hao et al. (2016b) proposed a novel process for fine particles abatement via heterogeneous condensation of water vapour coupling two impinging steams technique. Bao et al. (2017) reported that nearly all the fine particles could be activated and grow up to be larger droplets in the desulfurized flue gas by adding steam to form a supersaturated environment, and these droplets could be removed by the mesh wire demister. All the above studies had proved that the principle of condensation of water vapour could effectively promote the growth of fine coal-fired particles in flue gas.

At present, the large coal-fired power plants are generally equipped with wet flue gas desulfurization system, and the temperature of the outlet flue gas is between 313.15K ~ 333.15K, the flue gas is close to saturation state and it is easy to realize the construction of a supersaturated environment. Therefore, studying the condensation growth characteristics of coal-fired particles in supersaturated water vapour environment is of great significance for realizing the ultra-low emission of fine particulate matters in coal-fired power plants.

Based on the previous studies, a kinetics model was established for the growth of coal-fired particles by the condensation of water vapour. Additionally, the effects of operational parameters such as growth time, degree of saturation, gas temperature and particle number concentration, on particle growth were numerically studied. Then the results could provide theoretical support for removing of fine particles, which could be larger by using vapour condensation technology.

### PHYSICAL MODEL

#### Simplification Assumption

The researches on the fly ash fine particles of coal-fired power plants indicate that the fine particles in the flue gas are mostly spherical and the surface is smooth (Sun et al. 2015). In addition, the compositions of fine particles are silicon-aluminous minerals insoluble in water (Li et al. 2009).

Based on the above research results, the model calculation can be simplified by the following assumptions.

- 1. Coal-fired particles are regarded as spherical insoluble particles and the collision between particles is ignored.
- 2. At the beginning of steam condensation, the particles can be completely covered by the liquid and the number concentration of particles are considered to be constant.
- 3. The system is an adiabatic system, and the heat transfer process between steam and droplets is a quasi-static process.
- 4. The temperature is uniformly distributed inside the environment and dust-containing droplets, the temperature between droplets and flue gas is defined as the temperature difference.

#### Model of Condensation Growth Kinetics

The water vapour condenses on the surface of coal-fired

particles to form dust-containing droplets and the surface equilibrium steam pressure of droplets are:

$$P_{va} = P_{sat}(T_l) \exp\left(\frac{4s_l M_l}{RT_l r_l d_p}\right) \qquad \dots (1)$$

Where,  $P_{sat}$  is the droplet surface saturation vapour pressure, Pa;  $T_1$  is the temperature of droplet, K;  $\sigma_1$  is the surface tension of droplet,  $N \cdot m^{-1}$ ;  $M_1$  represents the molar mass of the droplet, kg·mol<sup>-1</sup>; R is the ideal gas constant,  $R = 8.314 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ ;  $\rho_1$  is the density of droplet, kg  $\cdot m^{-3}$ ;  $d_p$  is the diameter of droplet, m.

The surface tension and saturation vapour pressure of droplet are given by (Yu et al. 2014).

$$P_{sat}(T_l) = \exp(77.34491296 - \frac{7235.424651}{T_l} - 8.2 \ln T_l + 5.7113 \cdot 10^{-3} T_l) \qquad \dots (2)$$

$$s_l = 0.001 \exp(4.859191 - 1.951091 \cdot 10^{-3} T_l) \dots (3)$$

The density of droplet is a function of temperature, which is given by:

$$r_l = \frac{w_1}{w_2} \qquad \dots (4)$$

Where,

$$w_{1} = 999.83952 + 16.945176T_{c} - 7.9870401 \cdot 10^{-3}T_{c}^{2}$$
  
-4.6170461 \cdot 10^{-5}T\_{c}^{3} + 1.0556302 \cdot 10^{-7}T\_{c}^{4}  
-2.8054253 \cdot 10^{-10}T\_{c}^{5} ...(5)

$$w_2 = 1 + 1.687985 \cdot 10^{-2} T_c \qquad \dots (6)$$

$$T_c = T_l - 273.15$$
 ...(7)

The mass flux of the vapour diffusing to the droplet surface is written as (Heidenreich et al. 1995).

$$q_m = \frac{2pd_p M_v D_v (P_{v\infty} - p_{va})(1 + Kn_v)}{RT_l (1 + 1.71 Kn_v + 1.33 Kn_v^2)} \qquad \dots (8)$$

Where,  $M_v$  represents the molar mass of vapour, kg·mol<sup>-1</sup>;  $D_v$  is the diffusion coefficient,  $m^2 \cdot s^{-1}$ ;  $P_{v\infty}$  is the ambient vapour pressure, Pa;  $Kn_v$  is the Knusen number of vapour,  $Kn_v = 2l_v/d_p$ ;  $l_v$  is the vapour molecular mean free path, m; And (Fan et al. 2013):

$$D_{\nu} = 2.50 \times 10^{-3} \left( P_{cg} P_{cv} \right)^{1/3} \left( T_{cg} T_{cv} \right)^{5/12} \\ \left( \frac{1}{M_g} + \frac{1}{M_{\nu}} \right)^{1/2} \left( \frac{T_{\infty}}{\sqrt{T_{cg} T_{cv}}} \right)^{2.334} \frac{1}{P_{\infty}} \qquad \dots (9)$$

Where,  $P_{cg}$  and  $P_{cv}$  are the critical pressure of flue gas and steam, Pa;  $T_{cg}$  and  $T_{cv}$  are the critical temperature of the flue gas and steam, K;  $M_g$  represents the molar mass of flue gas, kg·mol<sup>-1</sup>;  $T_{\infty}$  is the temperature of flue gas, K;  $P_{\infty}$  is the total pressure of flue gas, Pa.

The growth rate of droplet diameter is defined as:

$$\frac{dd_p}{dt} = \frac{2q_m}{pd_p^2 r_l} \qquad \dots (10)$$

When the steam condenses, the latent heat is released to the droplet, causing the rise of droplet temperature. According to the law of conservation of energy, the raised droplet temperature is (Wen et al. 2014):

$$T_{l} = T_{\infty} + \frac{q_{m}L\left(1 + 1.71 K n_{g} + 1.33 K n_{g}^{2}\right)}{2p d_{p} l\left(1 + K n_{g}\right)} \qquad \dots (11)$$

Where, L represents latent heat of phase change,  $J \cdot kg^{-1}$ ; Kn<sub>g</sub> is the Knusen number of flue gas,  $Kn_g = 2l_g/d_p$ ;  $l_g$  is the molecular mean free path of flue gas, m;  $\lambda$  is the thermal conductivity of flue gas,  $W \cdot m^{-1} \cdot K^{-1}$ .

The rate of change of the ambient vapour pressure is:

$$\frac{dp_{v\infty}}{dt} = -\frac{RT_{\infty}}{M_v} \sum_{i=1}^K n_i q_{m,i} \qquad \dots (12)$$

Where, n is the number concentration of particles,  $m^{-3}$ ; the subscript i represents different intervals.

The release of latent heat of vapour will also cause the

rise of flue gas temperature, and the change rate of flue gas temperature is:

$$\frac{dT_{\infty}}{dt} = -\frac{RT_{\infty}L}{\left(P_{\infty} - P_{\nu\infty}\right)M_g c_{pg} + P_{\nu\infty}M_\nu c_{p\nu}} \sum_{i=1}^K n_i q_{m,i} \quad \dots (13)$$

Where,  $c_{pg}$  and  $c_{pv}$  are the constant pressure specific heat of flue gas and vapour, J·kg<sup>-1</sup>·K<sup>-1</sup>.

#### **Initial Size Distribution**

It is assumed that the initial particle size distribution of coal particle complies to log-normal distribution, in which the geometric standard deviation  $\sigma_{g0} = 1.5$ , average particle size  $d_{g0} = 0.25 \ \mu$ m. The number density function of the initial distribution for coal-fired particles is expressed as:

$$\frac{dn}{dd_p} = \frac{n_t}{\sqrt{2p} d_p \ln s_{g0}} \exp\left[-\frac{\ln\left(d_p / d_{g0}\right)}{2\ln^2 s_{g0}}\right] \qquad \dots (14)$$

Fig.1 shows the initial particle size distribution. Among the fine particle groups of the distribution, the particles with the diameters ranging from  $0.07 \,\mu\text{m}$  to  $0.84 \,\mu\text{m}$  account for 99.73% of the total particles.

#### **RESULTS AND DISCUSSION**

# The Evolution of Particle Size Distribution with Growth Time

In order to investigate the evolution of particle size distribution with growth time, we set the calculation conditions as



Fig. 1: Initial particle size distribution.

follows: the temperature of flue gas is 323.15 K, the number concentration of particles is  $10^6$ /cm<sup>3</sup>, the initial super saturation is 1.25. Fig. 2 shows the evolution of particle size distribution with time. It can be seen from Fig. 2 that with the prolongation of growth time for coal-fired particles in the super saturation vapour environment, the final particle size becomes larger and the distribution becomes more concentrated. When the growth time is 20 ms, almost all particle sizes are concentrated at  $3.33 \sim 3.87$  µm.

Fig. 3. shows the evolution of typical particle size and ambient vapour pressure with time. It can be seen that the process of particle growth is basically completed in the first 20 ms, fine particles larger than 0.05  $\mu$ m can grow to more than 3.33  $\mu$ m and the grown particles can be effectively removed by conventional dust removal equipment. The conclusion is consistent with the result of Heidenreich et al. (1995). In addition, it is found that as the growth time increases, the growth speed becomes slower. It could be explained



Fig. 2: Evolution of typical particle as a function of time.



Fig. 3: Evolution of typical particle size and ambient vapour pressure with time. (a) Evolution of typical particle size with time (b) Evolution of ambient vapour pressure with time

as follow: on the one hand, as the vapour condenses on the particle surface, the ambient vapour pressure decreases and the amount of condensable vapour in the environment is reduced, resulting in the reduction of condensation power. On the other hand, water vapour condenses on the surface of coal-fired particles and releases latent heat of phase transformation resulting in the increase temperature and equilibrium steam pressure of particle, which is conducive to growth of particles.

# Effects of Supersaturation on Condensation Growth of Particles

To research the effects of super saturation on condensation growth of particles, the calculation conditions are as follows: the temperature of flue gas is 323.15 K, the number concentration of particles is  $10^6$ /cm<sup>3</sup>, the growth time is 30 ms and the initial degree of saturation are set as 1.15, 1.20, 1.25 and 1.30, respectively. Fig. 4 shows the effects of super saturation on condensation growth of particles. As the increase of super saturation, the final diameter of particle increases and the range of particle size becomes narrower. This is because when the gas phase temperature is constant, the greater the super saturation of vapour, the higher the ambient vapour pressure and the larger vapour condensation driving force, which is conductive to the growth of coal-fired particle. Under the condition of superstation 1.3, the final diameter for coal-fired particles is ranging from 3.56 µm to 4.08 µm, which is consistent with the results of Wen et al. (2014).

# Effects of Flue Gas Temperature on Condensation Growth of Particles

In order to explore the effects of flue gas temperature on condensation growth of particles, we set the calculation conditions as follows: the number concentration of particles is 10<sup>6</sup>/cm<sup>3</sup>, the growth time is 30 ms, the initial saturation is set as 1.25 and the gas temperature are set as 313.15K, 318.15K, 323.15K and 328.15K, respectively. Fig. 5 shows the effects of flue gas temperature on condensation growth of particles. It can be seen that when the flue gas temperatures are 313.15K, 318.15K, 323.15K and 328.15K, respectively, the final diameters for particles are concentrated at 2.73~3.52 μm, 3.69~3.03 μm, 3.89~3.33 μm and 4.12~3.64 μm, respectively. When the degree of super saturation is constant, the higher the gas phase temperature, the larger the final diameter of particles after condensation growth. It could be explained that when the saturation of vapour is constant, the higher the temperature of flue gas is, the larger the amount of condensable vapour in the environment. Thereby, more steam can condense on particle surface, increasing the final size of the particle.

The wet desulfurization of coal-fired power stations produce high-humidity flue gas with a temperature ranging from 313.15K to 333.15K, only a small amount of steam is added to the flue gas to build an over-saturated environment, which is meaningful for phase change condensation to promote the growth of coal-fired particles.



Fig. 4: Effects of super saturation on condensation growth of particles.



Fig. 5: Effects of gas temperature on condensation growth of particles.



Fig. 6: Effects of particle number concentration on condensation growth of particles.

# Effects of Particle Number Concentration on Condensation Growth of Particles

To study the effects of particle number concentration on condensation growth of particles, the calculation conditions are as follows: the initial super saturation is 1.25, the temperature of flue gas is 323.15K, the growth time is 30ms and the number concentration of particles are  $4 \times 10^5$ /cm<sup>3</sup>,

 $6 \times 10^{5}$ /cm<sup>3</sup>,  $8 \times 10^{5}$ /cm<sup>3</sup> and  $1 \times 10^{6}$ /cm<sup>3</sup>, respectively. Fig. 6 shows the effects of particle number concentration on condensation growth of particles. It can be seen from Fig. 6 that the smaller the number concentration of particles, the better growth effect of particles. When the number concentration of fine particles is  $4 \times 10^{5}$ /cm<sup>3</sup>, the fine particles after growth are ranging from 4.58 µm to 5.01 µm. It could be explained as follow: when the flue gas temperature and initial super saturation are constant, the amount of condensable steam in the environment is certain. Increasing the number concentration of fine particles is bound to intensify the competition for steam among particles. Therefore, the amount of steam obtained by a single particle is reduced and the final diameter of particle after condensation growth will be smaller. Therefore, an appropriate supersaturated steam field should be constructed, according to the number and concentration of fine particles.

### CONCLUSION

A dynamics model was established for condensation of water vapour on the surface of coal-fired particles. The influences of operational parameters, including growth time, degree of saturation, temperature of flue gas and particle number concentration on particle growth were numerically investigated. The calculation results show that coal-fired particles can grow rapidly in the over saturated steam environment, the growth process can complete within a few tens of milliseconds, and the size distribution of fine particles becomes narrower after the growth. Increasing the initial super saturation and temperature of flue gas can increase the amount of condensable steam and enhance the driving force of condensation, which effectively promotes the condensation growth of particles. Additionally, increasing the number concentration of coal-fired particles will intensify the competition between particles for water vapour, which is not conducive to the condensation growth of particles.

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