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# The Study of Heterogeneous Condensation of Water Vapor on Submicron Particles in Cooled Tube by Population Balance Model

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The removal of submicron particles is becoming extremely important due to increasing serious air pollution in recent years. Heterogeneous condensation, as the prospective preconditioning technique, was paid more attention for its operability. This work is mainly to investigate the process of the heterogeneous condensation of water vapor in cooled tapered tube. The supersaturation environment of heterogeneous condensation was achieved by cooling the wall temperature of the tube. The Eulerian-Eulerian two-fluid approach was used to calculate the trajectory of the fluid in this physical model. The population balance model was used to simulate the growth process of particles in the flow field. It was found that the environment of particle enlargement was established when the temperature of the flue gas lower than the temperature of the wall surface. Particle growth was favoured by increasing residence time in cooled tube. When the initial concentration of particles is high, particles enlargement would be decreased due to insufficient water vapor under the same degree of supersaturation.

## 1. Introduction

Nowadays, the traditional dust removal equipment can remove 99% of the particulate matter in the flue gas, but only for quality removal. Indeed, the removal efficiency for the ultrafine particles of flue gas is still very low (Biswas, 2005). Therefore, the pre-treatment technology that is used to increase the size of ultrafine particles has been more and more attention (Mancuso, 2014). At present, the most common pre-treatment techniques include electronic reunion, chemical agglomeration, acoustic agglomeration and water vapor phase change coagulation. In this case, the water vapor phase change is a very promising method. The condensation of vapor on the surface of the fine particles is the main principle that allows the particles to grow in order to remove particulates through conventional equipment.
People began to study the heterogeneous vapor condensation since the last century. Fletcher put forward the classic heterogeneous nucleation theory in the 1950s. Tammaro et al. (2012) proposed the use of hot water and cold flue gas mixed to make the flue gas achieve supersaturation, and then investigate the growth of particles at different saturation conditions. Fan et al. (2007) proposed a numerical simulation method to predict the condensation results of steam on the basis of Fletcher's classical heterogeneous nucleation theory. Yang et al. (2009) analysed the heterogeneous nucleation of the various factors by adding steam to the system of wet flue gas desulfurization. Therefore, an important factor in studying heterogeneous nucleation is to construct a suitable supersaturation environment. This paper is intended to construct an environment by means of cooling the high temperature of flue gas, which heterogeneous nucleation is generated. The effects of these factors on heterogeneous nucleation were investigated, including the flow rate, the temperature of flue gas and the concentration of particulate matter in the flue gas.

## 2. Model

This work mainly does a research for the parameters in the process of the particle growth and coalescence process through the FLUENT software. Taking into account the operability of numerical simulation, researchers pay more attention on it. Vairo et al. (2014) used dispersion modelling to simulate the

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atmospheric emissions from a fossil fuel power station. Conventional numerical simulations for the removal of particulate matter are usually performed by using the Euler Lagrange method, which thought of gas as a continuous phase and discrete particles as discrete phases. However, this method cannot make a detailed analysis of the growth of particulate matter because the particles as discrete. Therefore, we consider them all as the continuous phase, using Eulerian-Eulerian two-fluid approach in this paper. The occurrence of heterogeneous nuclei is closely related to the supersaturation (Reiss. 1995), which is defined as the ratio of the partial pressure $P_V$ of the water vapor in the wet air to the partial pressure $P_{sat,T}$ of the water vapor in the saturated humid air (Mcdonald, 1974).

$$S = \frac{P_v}{P_{sat,T}} \tag{1}$$

The process of heterogeneous nucleation can be roughly divided into two parts: nucleation and growth. When the relative humidity is greater than 100 %, the water vapor begins to condense on the surface of the particulate matter. The nucleation rate in this process was given by the following formula:

$$J = \frac{2}{\rho_1}\sqrt{\frac{m_l \sigma_s}{2\pi}}\left(\frac{P_V}{k_B T}\right)^2 \cdot \exp\left[-\frac{\pi \sigma_s}{3 k_B T} D_{K,v}^2\right] \tag{2}$$

and

$$D_{\mathrm{k,v}} = \frac{4\sigma_s M_w}{\rho_l R_g T \cdot InS} \tag{3}$$

where $m_l$ is the mass of a vapor molecule; $k_B$ is Boltzmann constant; $\sigma_s$ is surface tension of the condensing species; $M_w$ is the molecular weight; $\rho_l$ is the liquid density; $R_g$ is the universal gas constant. $D_{k,v}$ is not the activation diameter but instead is a property of the condensing species and is equal to the diameter of a droplet of the condensing species in equilibrium with its vapor at saturation ratio, $S$, and temperature, $T$.(Susanne. 2005) From the above formula, it can be seen that higher supersaturation is needed when the particle size is smaller. But when the supersaturation is too high, homogeneous nucleation affects the efficiency of nucleation and increases the cost of nucleation.
The growth process of particles after nucleation can be described by the Kulmala equation (Fisenko. 2007) to investigate the relationship between the growth rate of particles and their supersaturation:

$$\frac{\mathrm{d}R}{dt} = \frac{S - S_a}{\rho R_p \left[\dfrac{R_g T}{\left\{\beta_m M_v D P_\infty \left[1 + \dfrac{(S+S_a)P_\infty}{2P}\right]\right\}} + \dfrac{S_a L^2 M_v}{\beta_l R_g K T^2}\right]} \tag{4}$$

Where $S$ is the supersaturation; $S_a$ is the supersaturation of the particle surface under the Kelvin effect; $\rho$ is the density of the particles; $D$ is the diffusion coefficient of the condensed vapor; $R_g$ is the gas constant, $L$ is the latent heat of vaporization; Thermal conductivity; $M_v$ is the mass of steam; $P_\infty$ is the saturated vapor pressure; $P$ is the total pressure; $\beta_m$, $\beta_l$ are the mass flow and heat flux correction coefficient. The condensation and growth rate increases with the increase of supersaturation. The higher degree of supersaturation can reduce the critical particle size of the occurrence of nuclear condensation, which accelerates more particles to coagulate and growth. Meanwhile it also can improve the particle coalescence rate and water vapor condensation on the surface of the particle number, so as to improve the particle removal efficiency. The PBM (population balance model) does not provide the nucleation and growth function, so compile the above Eq(2), (4) into udf, then put it into fluent to calculate the nucleation rate and growth rate of the particles.
In this paper, the model is simplified to two dimensions for convenience. Figure 1 shows the physical model. The model has a length of 0.1 m, an inlet diameter of 0.01 m, and an outlet diameter of 0.005 m.

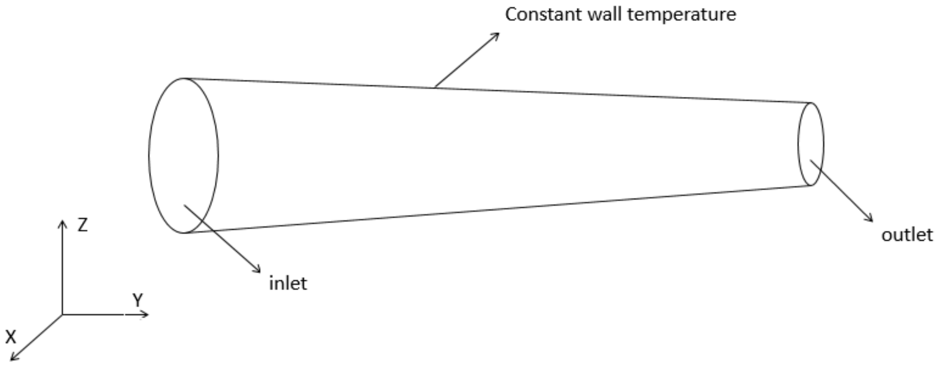



*Figure 1: Physical model*

## 3. Numerical simulation results and analysis

Compared with the cylindrical tube, this model can make improve the removal efficiency of particulate matter. When the inlet velocity is 1 m/s, the temperature of flue gas is 303 K, the temperature of wall surface is 288 K, the inlet initial particle size is $10^{-7}$ m, and its volume fraction is $10^{-5}$, the distribution of supersaturation and temperature in the tapered tube and cylindrical tube is shown in Figure 2.

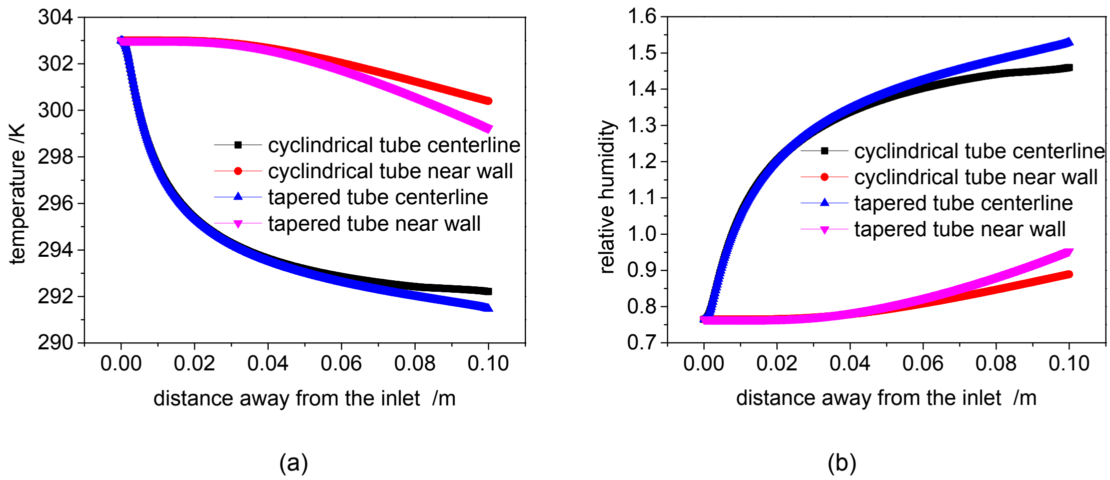


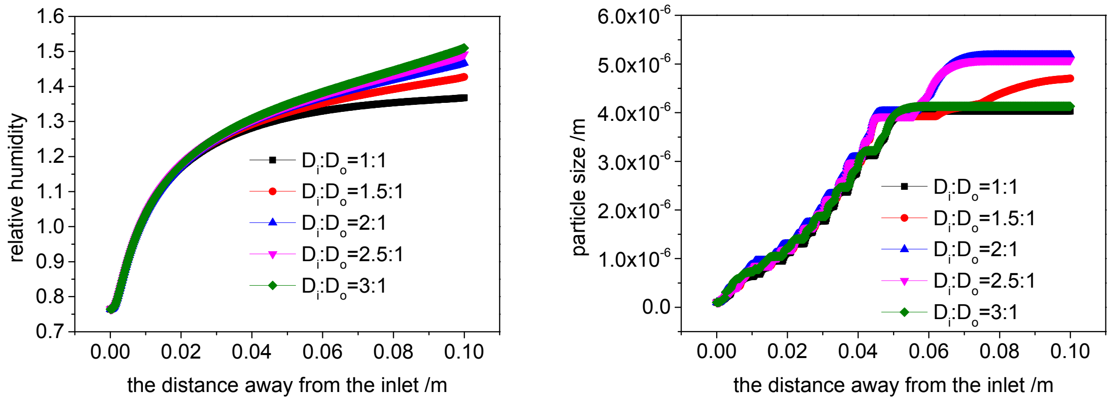

*Figure 2: The distribution of supersaturation and temperature of tapered tube and cylindrical tube*

From the temperature of the Figure 2a, it can be seen that the temperature decreases along the direction of flue gas flow, and the temperature at the centerline is higher than it near wall. The temperature drop in the tapered tube is higher than it in the cylindrical tube, so the relative humidity in the tapered tube is higher than it in the cylindrical tube, as we have seen in Figure 2b. Therefore, the tapered tube can provide a more suitable environment for the heterogeneous nucleation of the particulate matter under the same conditions.

### 3.1 Slope of Tube Wall

With a different slope of the tube wall, the growth of particulate matter is different. Figure 3 shows the simulation results at different slope of the tube wall when the inlet velocity is 1 m/s, the flue gas temperature is 303 K, the wall temperature is 293 K, the initial particle size is $10^{-7}$ m, and the volume fraction is $10^{-5}$. The $D_i$ : $D_o$ in Figure 3 means the ratio of the inlet diameter to the outlet diameter.
Figure 3a shows the distribution of supersaturation with different slope of tube wall. When the slope is larger, heat transfer effect is marvelous, so as to flue gas can achieve higher saturation. However, as can be seen from the Figure 3b, the growth of particulate matter does not show a direct proportional relationship with the supersaturation in this case. This is due to the growth of the particles is not only related to the supersaturation, but also to the residence time in the tube.

A lager slope of the tube wall leads to a shorter residence time. Therefore, the growth efficiency of particulate matter is best when the diameter ratio between the inlet and the outlet is 2: 1 in the course of this simulation.




(a) (b)

*Figure 3: The distribution of supersaturation and particle size with different slope of tube wall*

### 3.2 Volume Fraction

At a certain degree of supersaturation, the maximum size of the particulate matter that grows through heterogeneous nucleation is limited. The lager initial concentration of particulate matter, the worse the growth effect of particulate matter within a certain degree of supersaturation. Under the condition of different volume fraction, Figure 4 shows the distribution of particle size at the outlet when inlet velocity is 1 m/s, the temperature of flue gas is 303 K, the temperature of wall surface is 293 K, and an initial particle size of $10^{-7}$ m.

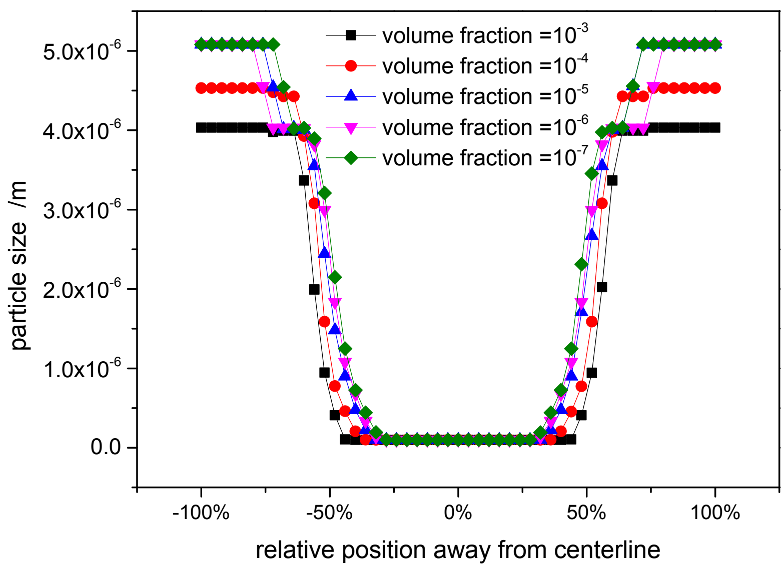
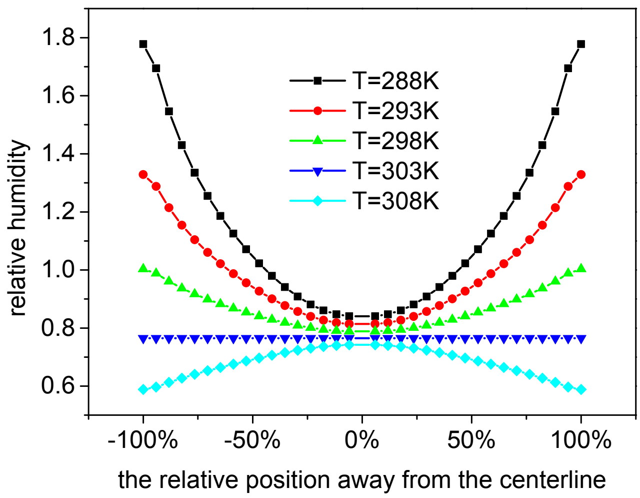



*Figure 4: The distribution of particle size with different volume fraction*

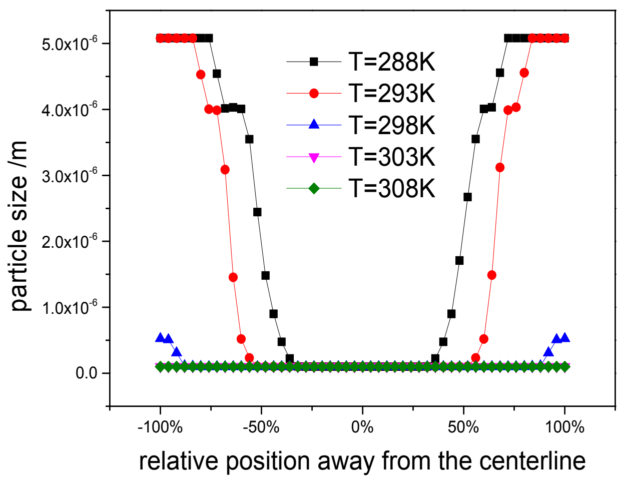
When the concentration of initial particulate matter is low, the growth of particulate matter is better at the outlet. The reason why is that the growth rate of the particles is constant when the supersaturation and time are fixed, high concentration of particulate matter consumes more water vapor in the flue gas, which causes the particle size at the same location is much lower than the particle size of the low concentration. In the case of a certain degree of supersaturation, the growth efficiency of the particulate matter will increase with the decrease of the initial particle concentration in a certain range.

### 3.3 Wall Temperature

When the wall temperature is lower than the flue gas temperature it will produce the effect of cooling flue gas, so the flue gas can achieve a higher degree of supersaturation. Figure 5a shows the supersaturation distribution in the tapered tube when the inlet particle size is $10^{-7}$ m, the flue gas velocity is 1 m/s, the flue gas volume fraction is $10^{-5}$, the flue gas temperature is 303 K and the wall temperature is different. When the wall temperature is lower than the flue gas temperature, the flue gas supersaturation rises due to the temperature drop, and when the wall temperature is higher than the flue gas temperature, the flue gas supersaturation will decrease due to the temperature rises. When the difference of temperature between the wall surface and the flue gas is large, the flue gas can achieve higher saturation.




(a)




(b)

*Figure 5: The distribution of supersaturation and particle size in different temperature*

Figure 5b shows the distribution of particle size under the condition of different temperature. It can be seen from the Figure 5 that the particle size will be larger in the location of high saturation. Particulate matter only grows when the relative humidity is greater than 100 %. As can be seen from Figure 5a, the relative humidity is larger close to the location near the wall, so the particles grow well at the same position.

## 4. Conclusion

Learning from the study in the past, it was often studied that factors affecting the growth of particulate matter within a certain supersaturated environment. In this paper, we discuss a method to make the flue gas reach the supersaturation state. We investigate the different temperature of wall surface, different slope of the tube wall and different initial concentrations to find the effect of the growth of particle based on this method. The following conclusions were drawn:

(1) The lower the wall surface temperature while the flue gas temperature in a certain range, the greater the over-saturation that can be produced, resulting in the better the steam phase change.
(2) In the same vertical plane, the farther away from the center of the tapering tube, the greater the temperature change, the greater the degree of supersaturation, the higher the maximum particle size concentration.
(3) The slope of the tube wall can improve the heat transfer of the gas, but the excess slope of the pipe will reduce the residence time and cause the effect of the growth of the particles to be reduced. Therefore, it is important to select the apt slope to simulate.
(4) In the case where the supersaturation has been determined, the growth efficiency of the particles increases in a certain range with the decrease of the initial concentration.

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