Effect of dustiness in atmospheric air on the formation and characteristics of condensation aerosol

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Abstract. In this work, the simulation of the formation process of condensation aerosol in atmospheric air is carried out. The influence of the initial supersaturation ratio and dustiness content on the formation mechanism and macroscopic characteristics of the aerosol is investigated.

1. Introduction

Condensation aerosol is a two-phase medium containing discrete particles of the liquid phase (droplets). This system can form if the vapor pressure exceeds the saturation pressure at the ambient temperature. This metastable state is called supersaturated vapor. Supersaturated vapor can condense using two mechanisms: the droplet formation due to homogeneous nucleation and heterogeneous condensation on the surface of solid particles. The simplest example of such a process is the formation of fog, in this case the supersaturated state is achieved due to isobaric cooling of atmospheric air. Also, condensation aerosol can be formed during adiabatic expansion of steam in the nozzle [1].

With intense evaporation near the interface, the vapor can be supersaturated [2] therefore bulk condensation is also possible. An analysis of the aerosol formation process under such conditions can be important for the investigation of droplet clusters [3], which is fundamental for understanding the mechanisms of propagation of harmful impurities and viruses.

In this paper, the effect of dustiness in atmospheric air on the formation and characteristics of aerosol is considered.

2. Formulation of the problem and mathematical description

The zero-dimensional problem of bulk condensation of steam is considered. At the initial time, steam is supersaturated, its partial pressure is higher than the saturation pressure corresponding to the ambient temperature \( T_0 = 300 \) K, the pressure of the vapor-gas mixture \( p_0 \) is equal to atmospheric one.

The mass of solid particles per unit volume is constant and is given by the value of \( \Phi \). The initial size distribution of particles is normal:

\[
f_0 = \frac{1}{\sqrt{2\pi D}} \exp \left( -\frac{r-M}{2D} \right),
\]

(1)
where $D$ is the variance and $M$ is the expected value. Normal distribution parameters are selected based on the regulations governing the content of dust in the air [4].

There can be a large number of droplets with different sizes and formation mechanism in considering system. Therefore, two droplet size distribution functions are used: $F$ for homogenous droplets and $f$ for heterogeneous droplets. The products $Fdr$ and $fdr$ determinate the number of droplets per volume unit, which size are in the range from $r$ to $r + dr$. The evolution of these distribution functions is described by the kinetic equations [5]:

$$\frac{\partial F}{\partial t} + \frac{\partial (\hat{F} F)}{\partial r} = I \delta (r - r_{cr});$$

$$\frac{\partial f}{\partial t} + \frac{\partial (\hat{f} f)}{\partial r} = 0.$$  \hspace{1cm} (2)

Here $t$ is time, $r$ is the droplet radius, $\hat{r}$ is the droplet growth rate, $I$ is the frequency of formation of critical droplets per volume unit (nucleation rate), $r_{cr}$ is the droplet critical radius, and $\delta$ is the Dirac delta function. The nucleation rate is calculated using classical nucleation theory [6]. Equations (2) and (3) are very similar, the only difference is on the right parts. In equation (3), the right part is equal to zero, because the number of drops formed as a result of condensation on solid particles in the system is constant. To solve these equations, the method of direct numerical solution presented in [7] is used.

The system includes four components: non-condensable gas, vapor, liquid and solid particles. Mass fraction of gas $Y_{gas}$ and solid particles $Y_{dust}$ do not change throughout the entire condensation process:

$$\frac{dY_{gas}}{dr} = 0;$$

$$\frac{dY_{dust}}{dr} = 0.$$  \hspace{1cm} (4)

The mass fraction of liquid $Y_{liq}$ increases due to the formation of a new phase nuclei and its growth, as well as due to heterogeneous condensation of vapor on solid particles. The increase in the mass of the liquid is calculated as follow:

$$\frac{dY_{liq}}{dr} = \frac{d}{dr} \left[ \rho_{liq} \left( \frac{4}{3} \pi \int r^3 dr - \frac{1}{\rho_{dust}} \Phi \right) \right],$$

where $\rho_{liq}$, $\rho_{\Sigma}$ and $\rho_{dust}$ are the density of the liquid, the multiphase mixture and the solid particles, respectively. The mass fraction of water vapor is determined from the equation of all system components:

$$\sum_i Y_i = 1.$$  \hspace{1cm} (6)

In this work, it is assumed that all droplets and solid particles have the same temperature, which changes due to release of the latent heat of the phase transition and interphase heat transfer:

$$\left( \rho_{dust} Y_{dust} c_{p,dust} + \rho_{liq} Y_{liq} c_{p,liq} \right) \frac{dT_d}{dt} = \left[ L - c_{p,vap} (T_d - T_m) \right] \rho_{liq} \hat{r} - q \cdot S_d,$$  \hspace{1cm} (7)

where $c_{p, dust}$, $c_{p, liq}$ and $c_{p, vap}$ are the heat capacities of the solid particles the liquid and vapor, respectively, $T_d$ and $T_m$ is the temperature of the droplets and the environment, $L$ is the heat of vaporization, $q$ is the interfacial heat flux, $S_d$ is the surface area of the droplets per volume unit, which is calculated as the second moment of the distribution function:
\[ S_d = 4\pi \int_{r_i}^r (F + f) r^2 dr. \] (9)

In the general case, the temperature of solid particles differs from the temperature of the liquid, but as a first approximation it is assumed that they are equal. Equation (8) takes into account that for condensation the vapor should be heated to the droplet temperature.

The change in the temperature of the mixture is described by the following energy equation:

\[ \rho m c_{p,m} \frac{dT_m}{dr} = qS_d. \] (10)

Here \( \rho_m \) and \( c_{p,m} \) are the density and heat capacity of the gaseous phase.

The droplet growth rate and interfacial heat flux are calculated using expressions for the free molecular regime [8]:

\[ \dot{r} = \frac{1}{\rho_{\text{liq}}} \left[ \frac{p_{\text{vap}}}{(2\pi R/\mu_{\text{vap}} T_m)^{1/2}} - \frac{p_r(T_d)}{(2\pi R/\mu_{\text{vap}} T_d)^{1/2}} \right], \] (11)

\[ q = 2p_{\text{vap}} \left( \frac{RT_m}{2\pi \mu_{\text{vap}}} \right)^{1/2} \frac{T_d - T_m + 2p_r(T_d)}{T_m} \left( \frac{RT_d}{2\pi \mu_{\text{vap}}} \right)^{1/2} - 2p_{\text{vap}} \left( \frac{RT_m}{2\pi \mu_{\text{vap}}} \right)^{1/2} + \frac{5}{4} \frac{w(p_r(T_d) + p_{\text{vap}})}{v_{\text{vap}}(p_{\text{vap}}/T_m + p_r(T_d)/T_d)}. \] (12)

\[ w = -\frac{\rho_{\text{liq}} \dot{R}}{\mu_{\text{vap}} (p_{\text{vap}}/T_m + p_r(T_d)/T_d)}. \] (13)

Here \( w \) is the transport speed of the vapor.

It is assumed that water vapor and non-condensable gas are ideal gases; therefore, the Mendeleev-Clapeyron equation of state is used to close the system of equations (2) - (13).

**Results and discussion**

Calculations are carried out for supersaturated steam in atmospheric air, which also contains solid particles. The supersaturated ratio of water vapor \( S_0 = p_{\text{vap}} / p_r(T_m) \) at the initial time is varied in the range from 1.25 to 4.5, and the content of solid particles \( \Phi \) is from 0.01 to 1 mg/m\(^3\). The calculation is continuing while the relative temperature difference between gaseous phase and droplets is greater than 0.1%. The evolution of the homogenous droplets size distribution function is shown in figure 1(a). At the initial stage, the nuclei of a new phase are formed (curves 1 and 2 in figure 1(a)), then, as the supersaturation decreases, the nucleation rate decreases, and the distribution function changes mainly due to the condensed particles growth (curves 3 and 4 in figure 1(a)). By the time moment corresponding to equilibrium between the liquid and vapor phases, the distribution function takes its final form (curve 5 in figure 1(a)). The number of drops formed as a result of heterogeneous condensation on solid particles does not change, therefore the distribution function \( f \) moves to the region of large radius throughout the entire process of condensation relaxation (figure 1(b)).

At the beginning of bulk condensation, the droplet temperature \( T_d \) rapidly increases due to active vapor condensation on their surface (figure 2). The growth rate decreases over time (figure 3) due to decrease of supersaturation, and the temperatures of the droplets \( T_d \) and the gaseous phase \( T_m \) equalize due to interphase heat transfer (figure 2).
Figure 1. The evolution of size distribution functions $F$ (a) and $f$ (b) at $S_0 = 2.75$ and $\Phi = 0.1 \text{ mg/m}^3$. $1 - 0.02 \mu s$, $2 - 1 \mu s$, $3 - 10 \mu s$, $4 - 25 \mu s$, $5 - 4746 \mu s$.

Figure 2. Time depends of droplet temperature (dash curve) and gas phase temperature (solid curve) at $S_0 = 2.75$ and $\Phi = 0.1 \text{ mg/m}^3$.

Figure 3. Time depends of homogenous (dash curve) and heterogeneous (solid curve) average relative radius at $S_0 = 2.75$ and $\Phi = 0.1 \text{ mg/m}^3$.

For clarity of the results, the value $\Omega$ is introduced, which is the ratio of the number of heterogeneous droplet to the total number of drops:

$$\Omega = \int_{r_c}^{r} dr \left( \int_{r_c}^{r} (F + f) dr \right)^{-1}$$

(14)

With an increase in the supersaturation ratio, the number of droplets formed by homogeneous nucleation increases greatly due to increase of nucleation rate. However, at $S_0 < 2.5$, the number of such droplets is negligible in comparison with the number of drops are formed by heterogeneous condensation on solid particles (figure 4). With an increase of the dust concentration in the air, the total surface for heterogeneous condensation increases, therefore the supersaturation ratio decreases faster and number of homogeneous droplets decreases.
Figure 4. Dependences of the ratio heterogeneous droplet to the total number of droplets on the initial supersaturation for different contents of solid particles.

The droplet size at the end of the condensation process is determined by two factors: the duration of the process and the intensity of condensation on the surface. Accordingly, with an increase in the initial supersaturation ratio, the growth rate of drops increases, and it takes for the system to reach thermodynamic equilibrium decreases. At low supersaturation $S_0 < 3$, the intensity of condensation on the surface increases faster than the duration of process decreases; therefore, the droplets reach large sizes (figure 5). With a subsequent increase in water vapor supersaturation, the duration of the condensation process rapidly decreases due to intense homogeneous nucleation (figure 5). An increase in the concentration of solid particles also slightly reduces the volumetric condensation time, since the total surface area for heterogeneous condensation increases. However, at high supersaturation, this effect is practically leveled out (figure 5). The average radius of heterogeneous droplets at the end of the process is somewhat larger than that of homogeneous ones.

Figure 5. Dependences of the average radius of homogeneous (a) and heterogeneous droplets (b) on the initial supersaturation for different contents of solid particles.
Conclusion
The characteristics of droplet condensation aerosol formed in atmospheric air are investigated. It is shown that, at a low initial supersaturation ratio \( S_0 < 2.5 \), the droplets are mostly formed due to heterogeneous vapor condensation on the surface of solid particles contained in the air. On the other hand, at \( S_0 > 3 \), the number of droplets formed as a result of homogeneous nucleation significantly exceeds the number of heterogeneous droplets. The content of solid particles in the air has little effect on the size of homogeneous and heterogeneous droplets at high supersaturation ratio.

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References
[1] Hou D, Jiang W, Zhao W, Bian J, Liu Y and Lai X 2018 Chem. Eng. Process. 133 128-136
[2] Anisimov S I, Imas Ya A, Romanov G S and Khodyko Yu V 1970 Deistvie izlucheniya bol’shoi moshchnosti na metally (The Effect of High Power Radiation onto Metals) (Moscow: Nauka)
[3] Fedorets A 2004 JETP Letters 79 372-374
[4] Hygienic standards GN 2.1.6.2604-10 2010 Maximum permissible concentrations (MPC) of pollutants in the atmospheric air of populated areas
[5] Hulburt H M and Katz S M 1964 Some problems in particle technology: A statistical mechanical formulation Chem. Eng. Sci.19555
[6] Kashchiev D 2000 Nucleation. Basic Theory with Applications (Oxford: Butterworth-Heinemann)
[7] Kortsensteyn N M, Samuilov E V and Yastrebov A K 2009 Int. J. Heat Mass Transfer 52 548
[8] Kortenshteyn N M and Yastrebov A K 2011 Int. J. Heat Mass Transfer 55 1133