Numerical simulation of submicron particles formation during the combustion of coals, taking into account coagulation and dust content of combustion products

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Abstract. Homogeneous–heterogeneous bulk condensation of potassium sulfate vapor has been numerically simulated in a dusty vapor–gas flow of coal combustion products upon their cooling along a technological path. A closed model that we have proposed for the formation of submicron particles in coal combustion products has been employed. Data on the concentration of particles formed at varied parameters of heterogeneous condensation sites have been obtained. Variations in the relative contributions of the homogeneous and heterogeneous mechanisms with variations in flow dustiness have been considered. Data on the influence of coagulation processes on the parameters of submicron particles resulting from coal combustion have been presented.

1. Introduction
The content of ecologically hazardous submicron particles in the atmosphere is subject to control in the Russian Federation [1, 2]. Limitations on the concentration of such particles are present in quality standards of ambient air of other countries, including the United States [3]. In the People’s Republic of China, the problem of reducing pollutant emissions into the atmosphere has acquired the high-priority status in national policy, which is evident from the introduction of a plan for the prevention and control of air pollution [4].

The emission of submicron particles upon coal combustion is a source of the aforementioned type of atmospheric pollution. In this case, the hazard is created by not only the particles themselves, but also the condensation of different hazardous substances, e.g., some toxic microelements contained in coals [5–7], on their surface.

The realization of the complex—thermodynamic and kinetic—approach in [8, 9] has made it possible to consider the effect of the content of aluminosilicates of volatile elements (potassium and sodium) on the parameters of condensation aerosols for various types of coals with different ash compositions. Also, this approach can be used to consider the possible influence of dustiness of coal combustion products and coagulation processes on the parameters of the condensation aerosols.

The object of this study is the homogeneous–heterogeneous bulk condensation in a dusty flow of coal combustion products with allowance for coagulation processes. The dustiness is caused by the presence of volatile ash resulting from the combustion of coal.
2. Mathematical model
We considered a stationary one-dimensional flow of dusty products of combustion in a channel at a constant velocity and preset axial temperature gradient, which simulated the cooling of combustion products in a technological path. It was assumed that the sizes of dust particles and droplets allowed us to use a single-velocity model, while the low concentration of condensing components in the combustion products made it possible to use a single-temperature approximation, under which the temperatures of the droplets and the gaseous phase are equal. The model used for the formation process of submicron particles (droplets) in coal combustion products comprised the following features: (1) formation of a condensable component (potassium sulfate) in the gaseous phase under the approximation of thermodynamic equilibrium and (2) formation of a potassium sulfate aerosol via the homogeneous–heterogeneous condensation with account of the process kinetics.

The driving force of the process of condensation is an increase in the partial pressure of a condensed component relative to an equilibrium value at a specified temperature, which is characterized by the degree of supersaturation. As applied to the case under consideration, the supersaturation ratio can be written in the form

\[ s = \frac{N_{K,SO_4}}{N_{K,SO_4}^e} \]  

(1)

Here, \( N_{K,SO_4} \) is the current number of moles of potassium sulfate in a gas phase, which corresponds to single-phase (with frozen condensation) thermodynamic equilibrium in the gas phase (an analog of partial vapor pressure), and \( N_{K,SO_4}^e \) is the number of moles of potassium sulfate in the gas phase, which corresponds to two-phase thermodynamic equilibrium in the system (an analog of saturated vapor pressure). At each step of the numerical simulation of bulk condensation kinetics, the degree of supersaturation was calculated as follows. The temperature dependence was obtained for the denominator of Eq. (1) in [8] from the calculated data of the thermodynamic stage of the complex approach. The law of mass action and material balance for the main components (for example potassium-containing components: KOH and K2SO4) in the gas phase without condensation in the temperature range of interest are used for determining the numerator of expression (1) [8].

As in [10], the homogeneous–heterogeneous condensation kinetics was described on the basis of the fact that two groups of droplets are present in the flow: 1) microdroplets resulting from homogeneous nucleation in the bulk of the vapor–gas mixture and 2) macrodroplets resulting from the vapor condensation on dust particles. The processes of the formation and growth of microdroplets are described by the kinetic equation, which, in the case of the homogeneous condensation in a one-dimensional stationary flow with no account taken of coagulation, has the following form (see, e.g., [11]):

\[ u \frac{\partial f}{\partial x} + \frac{\partial (r f)}{\partial r} = \frac{I}{\rho_x} \delta (r - r_c), \]  

(2)

where, \( f \) is the particle mass size distribution function normalized with respect to the number of droplets in unit mass of the vapor–gas–droplet mixture, \( u \) is the flow velocity, \( x \) is the coordinate along the flow axis, \( r \) is the droplet radius, \( r_c \) is the rate of particle growth, \( I \) is the rate of nucleation, \( \rho_x \) is the density of the vapor–gas–droplet mixture, \( \delta \) is the Dirac delta function, \( r_c \) is the critical droplet radius.

For macrodroplets, the kinetic equation has the form of

\[ u \frac{\partial f_M}{\partial x} + \frac{\partial (r f_M)}{\partial r} = 0 \]  

(3)

Here, \( f_M \) is the macrodroplet size distribution function. In contrast to Eq. (2), the right-hand side of Eq. (3) is equal to zero because the number of macrodroplets is constant and equal to the number of heterogeneous nucleation sites (dust particles). The results of the numerical study [10] have shown
that the allowance for the polydispersity of the heterogeneous nucleation sites leads to a change in the number concentration of droplets and the condensate mass fraction within 10% relative to the monodisperse approximation at the same mass fraction of dust particles. In this work we used the monodisperse approximation.

The expression, which determines the kinetics of vapor condensation on dust particles, is as follows:

\[
\frac{dc_{\text{het}}}{dx} = \frac{4\pi n_p r_p^2 \hat{r}_{\text{p}}}{\rho_u u}
\]

(4)

Here, \(c_{\text{het}}\) is the mass fraction of the condensate formed on the dust particles; \(n_p\) and \(r_p\) are the number of the dust particles in unit volume and their radius, respectively; and \(\hat{r}_{\text{p}}\) is the rate of condensation growth of the dust particles, which is determined by the Fuchs equation [12]:

\[
\hat{r}_p = \frac{\alpha (p_v - p_s)}{\rho_v \sqrt{2\pi R T / \mu_v}} \left( 1 + \frac{\alpha}{D \sqrt{2\pi R T / \mu_v}} r_p + \langle \ell \rangle \right)^{-1}
\]

(5)

where \(\alpha\) is the condensation coefficient; \(p_v\) and \(p_s\) are the vapor partial pressure and the saturation pressure, respectively; \(R\) is the gas constant; \(\mu_v\) is the vapor molar mass; \(D\) is the diffusion coefficient; and \(\langle \ell \rangle\) is the mean free path of vapor molecules.

Vapor concentration was calculated by the material balance equation

\[
\frac{dc_v}{dx} = \left( \frac{dc_{\text{hom}}}{dx} + \frac{dc_{\text{het}}}{dx} \right),
\]

(6)

where \(c_{\text{hom}} = \rho_v / \rho_u\) is the mass fraction of the condensate formed by the homogeneous mechanism.

Also, the effect of flow dustiness may be realized via the coagulation mechanism upon the collisions of submicron droplets with dust particles. When estimating the effect of coagulation processes, we also took into account the collisions of droplets with each other (under the approximation of the Brownian coagulation of monodisperse spherical particles by analogy with [13,14]) and with dust particles (collisional coagulation). The coagulation-induced decrease in the number of droplets was calculated via the following expression:

\[
u \frac{dn_p}{dx} = -\left( K_0 n_p^2 / 2 + K_1 n_p n_u \right)
\]

(7)

where \(K_0\) is the Brownian coagulation constant and \(K_1\) is the collisional coagulation constant. Taking into account the approximate character of the approach, the calculations were performed at constant value \(K_0 = 6 \times 10^{-10} \text{m}^3/\text{s}\), which made it possible to match calculated and experimental data in [15]. The value of \(K_1\) was determined taking into account the fact that the size of dust particles (10 \(\mu\)m and more) is substantially larger than the size of submicron droplets:

\[
K_1 = \pi r_p^2 v_{\text{rel}}
\]

(8)

where \(v_{\text{rel}}\) is the velocity of collisions between droplets and dust particles. The correct calculation of this value is a separate complex problem (see, e.g., [16]). In this work, the effect of the collisional coagulation was estimated using \(v_{\text{rel}}\) values equal to 1 and 10% of flow velocity \(u\). As follows from expressions (7) and (8), the dustiness of the flow affects the coagulation of the formed droplets via complex \(n_p r_p^2\).

3. Calculations results

One of the coals considered in [8] was used as an object of simulation. Numerical simulation data on the formation of submicron particles (droplets) in the combustion products of coal Yanzhou (People’s
Republic of China) upon the homogeneous–heterogeneous condensation of potassium sulfate are presented in figures 1–4.

Figure 1. Variations in vapor concentration (solid curves) and temperature (dashed curve) along the channel axis at different values of $n_pr$: (0) 0, (1) 250, (2) 1000, and (3) 1500.

Figure 2. Variations in the supersaturation ratio (solid curves) and temperature (dashed curve) along the channel axis at different values of $n_pr$: (0) 0, (1) 250, (2) 1000, and (3) 1500.

Figure 1 illustrates vapor concentration variations in the zone of homogeneous–heterogeneous condensation at different values of parameter $n_pr$ and a fixed rate of temperature variation (480 K/s). The data on the purely homogeneous case are presented for comparison. Two regions are distinctly seen in the curves for a decrease in the vapor concentration: the initial region, which is characterized by a smooth variation in the vapor concentration upon heterogeneous condensation, and the final region, which is characterized by an abrupt change in the vapor concentration due to homogeneous condensation. As $n_pr$ increases, the length of the zone of the heterogeneous condensation on the duct particles and the contribution of this process to the vapor loss increase. At the same time, the zone of the homogeneous condensation shifts toward lower temperatures and vapor concentrations and, simultaneously, toward higher degrees of supersaturation (figure 2).

The number of droplets resulting from homogeneous nucleation increases (figure 3, solid curves) with a simultaneous decrease in their mass (figure 4).

The results of calculating the droplet concentration with allowance for the coagulation processes are presented in figure 3 by the dashed and dash-dot curves. The dashed curves represent the data of the calculations performed taking into account only the Brownian coagulation. The dash-dot curve reflects the data of the calculations carried out with account of both the Brownian coagulation and collisional coagulation at $v_{rel} = 0.1u$. At $v_{rel} = 0.01u$, the effect of the collisional coagulation is inconspicuous against the background of the Brownian coagulation. The effects of these processes are seen to be weak for both the dust-free and dusty flows.

4. Conclusions

In these studies, data on the parameters of submicron particles formed upon coal combustion have been obtained taking into account the effect of flow dustiness. The assumption of the ideal wettability of the heterogeneous condensation sites (dust particles) has yielded the upper estimate of their effect on the process of bulk condensation. It has been revealed that flow dustiness leads to a decrease in the mass concentration of submicron particles due to the partial condensation of vapor on the dust particles. At the same time, the number concentration of the submicron particles increases and their size decreases, and this circumstance must be taken into account when planning the trapping of such particles.
Figure 3. Variations occurring along the channel axis in the concentrations of droplets resulting from homogeneous nucleation with no regard to coagulation (solid curves) and with regard to coagulation (only Brownian (dashed curves) and Brownian and collisional (dash–dot curves) at different values of $n_{p}r_{p}$: (0) 0, (1) 250, (2) 1000, and (3) 1500.

Figure 4. Variations occurring along the channel axis in condensate mass fractions upon homogeneous (solid curves) and heterogeneous (dashed curves) condensation at different values of $n_{p}r_{p}$: (0) 0, (1) 250, (2) 1000, and (3) 1500.

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