

Dynamics of deposition of ultrafine aerosol created by pulse method

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Due to the danger of emergency emissions of toxic gases, the problem of their rapid neutralization arises. A method for pulsed spraying of adsorbent particles in a polluted environment has been developed. A mathematical model of ultrafine aerosol deposition is proposed, taking into account the processes of particle propagation, deposition, and coagulation. The model estimates the total surface of particles.

Keywords: ultrafine aerosol, pulsed spraying, deposition, coagulation, particle surface.

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Rapid purification of indoor air from hazardous substances is required in certain scenarios: fires, chemical leaks at industrial plants, bacterial and viral contamination [1]. The speed of air purification is critical in such cases. Thus, the issues of air purification from accidental emissions necessitate the development of new methods for removal of hazardous substances. Specifically, a method for neutralizing gas emissions by instantaneous pulsed generation of an ultrafine aerosol based on nanostructured powder particles has been proposed in [2]. Such particles with a large specific surface area have the capacity to adsorb toxic gases. In addition to adsorption, photocatalytic oxidation initiated by ultraviolet radiation is used. In this case, gases are adsorbed on the surface of a nanosized solid semiconductor material and decompose under ultraviolet irradiation [3–5].

The surface area of particles is the crucial parameter affecting the efficiency of gas adsorption by powder particles. Adsorption proceeds exactly on the surface of particles (including the nanopore system). Aerosol particles spread in space and get deposited on the walls and floor of a room. This is the reason why the concentration of particles and their total surface area needed for gas adsorption decrease gradually.

The aim of the present study is to examine the dynamics of variation of the total surface area of particles of an ultrafine adsorbing aerosol (produced by pulsed spraying) with account for the polydispersity of this aerosol and the processes of diffusion, deposition, and coagulation of particles proceeding simultaneously.

Let us consider an aerosol cloud of particles with diameter D smaller than $10\ \mu\text{m}$: a polydisperse system with a given initial particle size distribution function $f_0(D)$. The size of the particle cloud at the initial moment is much smaller than the characteristic room dimension H (point source approximation); the source is located in the center of a cubic chamber with edge H . This formulation of the problem corresponds to the case of pulsed spraying: the primary aerosol cloud is produced almost instantly; the particle size is small due to fragmentation under explosive spraying conditions; small particles are stopped

in air within a fraction of a second, traveling a distance shorter than 5 cm [2]. The spread of particles in space is driven by convective/turbulent diffusion and accompanied by gravitational deposition and deposition on the walls (ceiling). The particles are considered to be spherical. When particles collide with each other, they coagulate; when they collide with surfaces, they remain there.

It is known that diffusion coefficient k_D is proportional to absolute temperature T and inversely proportional to viscosity of air μ and characteristic particle diameter D : $k_D = k_{D0} \frac{T}{\mu D}$, where coefficient k_{D0} is a free parameter of the model.

Analytical expressions for the deposition of monodisperse aerosol particles on walls and gravitational deposition were obtained in [2]. In the general case, mass m_p of particles deposited at time t is

$$\frac{m_p(t)}{m_p(0)} = 1 - \exp(-\gamma t). \quad (1)$$

The deposition rate coefficient depends in a nonlinear fashion on the particle diameter:

$$\gamma(D) = \frac{u_s}{H} + \beta = \frac{\rho_p D^2}{18\mu H} g + \frac{\beta_0 k_{D0}}{H} \frac{T}{\mu D}, \quad (2)$$

where γ is the deposition rate coefficient, u_s is the rate of Stokes deposition, $u_s = \rho_p D^2 g / 18\mu$, ρ_p is the particle density, g is the gravitational acceleration, wall deposition coefficient β is proportional to the diffusion coefficient and inversely proportional to the distance to the walls: $\beta = \beta_0 k_D / H$, and β_0 is a free parameter of the model.

The diameter corresponding to the minimum of function $\gamma(D)$ is

$$D_{\min} = \sqrt[3]{\frac{9\mu\beta_0 k_{D0}}{(\rho_p - \rho)g}}. \quad (3)$$

An aerosol with particles of this diameter will remain in air for the longest period of time.

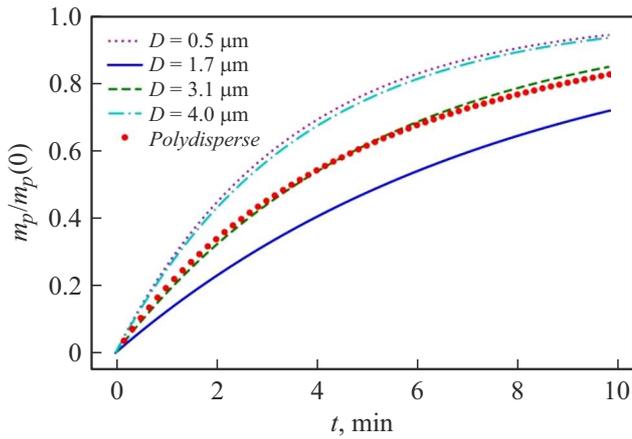


Figure 1. Temporal variation of the relative mass of deposited particles.

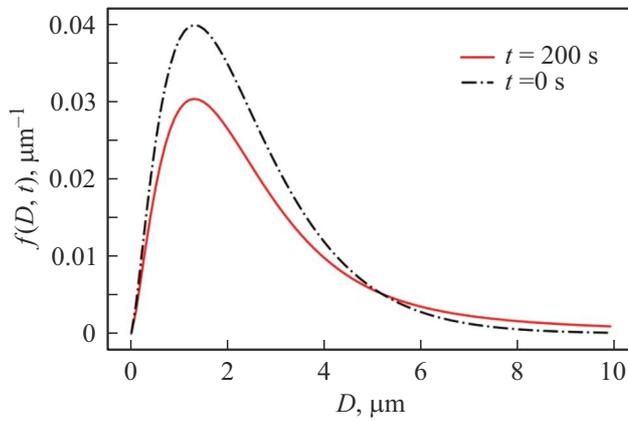


Figure 2. Variation of the particle size distribution function due to coagulation.

Equation (1) for a polydisperse aerosol may be written as

$$\frac{m_p(t)}{m_p(0)} = \int_0^{\infty} f_0(D) [1 - \exp(-\gamma(D)t)] dD. \quad (4)$$

The particle sizes follow a given initial distribution (gamma distribution with parameters α and b): $f_0(D) = aD^\alpha \exp(-bD)$, $a = \beta_1 b^{\alpha+1} / \Gamma(\alpha + 1)$, where $\Gamma(x)$ — gamma function, $\alpha = 1.4$, $b = 1 \mu\text{m}^{-1}$, and the characteristic size (Sauter diameter) is $D_{32} = 4.4 \mu\text{m}$.

Let us use the Smoluchowski approach to introduce coagulation and characterize the variation of particle size distribution function $f(D, t)$:

$$\frac{\partial f(D, t)}{\partial t} = I_1 + I_2. \quad (5)$$

Term I_1 in (5) represents the reduction in number of particles with diameter D per unit time as a result of collision with particles of diameter D_1 :

$$I_1 = -f(D, t) \int_0^{\infty} K(D, D_1) f(D_1, t) dD_1, \text{ where } K(D, D_1) \text{ is}$$

the probability of collision of particles with diameters D and D_1 in unit time. The probability of collision of particles is proportional to their cross sections: $K(D, D_1) = k_p(D^2 + D_1^2)$. The higher the value of proportionality coefficient k_p is, the higher is the coagulation intensity. Term I_2 characterizes the increase in number of particles with diameter D due to collisions of particles with smaller diameters $D_2 = \sqrt[3]{D^3 - D_1^3}$ and D_1 :

$$I_2 = \frac{1}{2} \int_0^D K(D_2, D_1) f(D_1, t) f(D_2, t) dD_1.$$

The initial conditions for Eq. (5): at $t = 0$ $f(D, 0) = f_0(D)$.

The variation of size of particles due to coagulation leads to a change in their free surface. Size effects induce significant changes in the rate of physical and chemical processes in aerosols [6].

The mass of particles remaining in air is proportional to the cube of their diameter, while their surface area is proportional to the diameter squared. Therefore, with (4) taken into account, the relative total surface area of particles in air is given by

$$\begin{aligned} \frac{S_p(t)}{S_p(0)} &= \left(1 - \frac{m_p(t)}{m_p(0)}\right)^{2/3} \\ &= \left(\int_0^{\infty} f(D_p) \exp(-\gamma(D_p)t) dD_p\right)^{2/3}. \end{aligned} \quad (6)$$

Here, $S_p(t)$ is the particle surface area at time point t and $S_p(0)$ is the initial particle surface area.

The parameters of the particle size distribution function were determined in the experiment on pulsed spraying of titanium dioxide powder [1]: $\alpha = 1.4$, $b = 1 \mu\text{m}^{-1}$. The free parameters of the model were determined based on experimental data. They were $\beta_0 = 0.025 \text{m}^{-1}$ and $k_{D0} = 3 \cdot 10^{-15} \text{H} \cdot \text{m/K}$.

Figure 1 presents the dynamics of variation of the relative mass of deposited particles calculated for particles of different diameters in accordance with the monodisperse model and for polydisperse model (4). Particles with diameters of 0.5 and $4 \mu\text{m}$ have approximately equal deposition rates, but particles with a diameter of $0.5 \mu\text{m}$ get deposited on the walls, while larger particles with $D = 4 \mu\text{m}$ are deposited on the floor. Particles with a diameter of $1.7 \mu\text{m}$ (corresponds to minimum diameter D_{\min} (3)) have the lowest deposition rate. The results of deposition calculations with the polydisperse model and the monodisperse model with a particle diameter corresponding to the volume-average diameter of the polydisperse distribution ($3.1 \mu\text{m}$) are virtually the same. Thus, a monodisperse model with the particle size corresponding to the volume-average diameter may be used in particle deposition calculations, which simplifies the process of estimation.

Figure 2 illustrates the change in the particle size distribution function due to coagulation ($k_p = 0.004 \mu\text{m}^{-2}$).

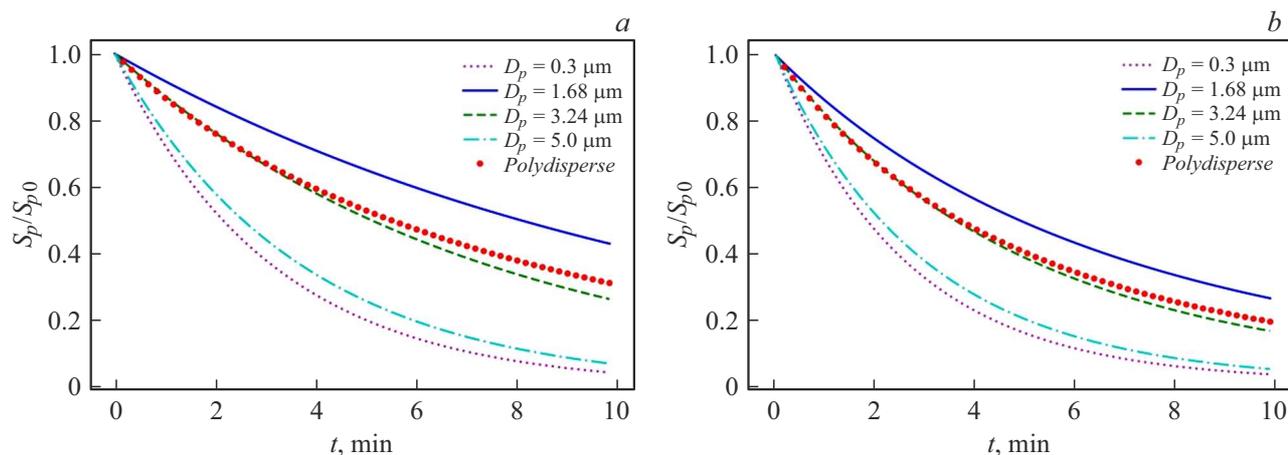


Figure 3. Relative total surface area of particles as a function of time. *a* — With deposition taken into account; *b* — with deposition and coagulation taken into account.

Figure 3 shows the time dependence of the relative surface area of particles calculated with the process of deposition and coagulation taken into account.

Calculations reveal that the particle surface area available for adsorption and chemical transformations is reduced significantly within 10 min (especially under intense coagulation). The reduction in surface area by the ninth minute for the model polydisperse distribution considered here is 60% due to deposition alone and 80% if coagulation is taken into account.

Thus, a mathematical model of the dynamics of deposition of an ultrafine aerosol produced by pulsed spraying was proposed. Time dependences of the relative mass of deposited aerosol particles, particle concentration, their dispersion, and surface area were obtained. It was demonstrated in model calculations for polydisperse titanium dioxide powder with a characteristic size of $4.4\ \mu\text{m}$ that the surface area of particles available for adsorption drops by 60–80% within a few minutes.

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Conflict of interest

The authors declare that they have no conflict of interest.

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