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Model of Absorption of Pollutants from Atmosphere by a Rain

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Abstract—The aim of this study was to create a mathematical model of absorption of pollutants from atmosphere by a rain. The speed, acceleration, established speed of drops depending on time and height taking into account the air's density were calculated. The process of absorption solids from atmosphere by drops with use of an efficiency of inertial catching of solids was considered. The dynamic absorption of gaseous pollutants was calculated. The results of the dynamic purification of the atmosphere from solids and sulfur dioxide were represented.
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Pollution of the atmosphere reached its record high within 650 thousand years [1]. This is due to the global human activity which alters the composition of the atmosphere. The world community is directing its efforts to reduce and limit emissions of pollutants into the atmosphere. Cleaning and restoration of the atmosphere itself go in a natural way. Precipitation is a natural way of cleaning the air from any kind of pollutants. It has long been known that the air is clean and fresh after rains. Clean air is one of the most important indicators of the ecological state of the environment. After the rain environmental conditions, even in large metropolitan areas of the world become significantly improved [2, 3]. The concentration of contaminants is 2.5–3 times lower than established standards. The content of sulfur dioxide, toluene and benzene in the air falls below acceptable limits. Thus, atmospheric precipitates are a natural phenomenon purifying the air from pollutants, dust and other solids.

General problems of water entering the atmosphere, condensation and formation of clouds and precipitation formation are well studied [4]. However, many processes, such as the dynamics of motion of rain towards the earth, the absorption of pollutants during the movement of precipitants, evaluation of residual concentration of pollutants in the air, the dependence of these processes on the intensity and duration of rainfall have not been considered.

The present study aims to partly fill this gap and to assess the dynamics of the decline the concentrations of pollutants in the atmosphere depending on the intensity and duration of rainfall.

MODEL

A model of the movement of raindrops and the absorption of pollutants from the atmosphere has been worked out. The model allows to calculate the absorbed solids and pollutants, depending on the droplet size, intensity and duration of rain.

The model consists of three blocks: "Movement", "The absorption of solids" and "Absorption of gaseous contaminants".

Assumptions made in the model:

(A) acceleration of gravity is 9.8 m s^{-2} (the error for the altitude of 5 km is less than 0.18%);

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(B) dependence of the air characteristics on temperature is not taken into account (the calculation is made for the temperature 14°C);

(C) drop shape is spherical (the deformation at dropping is not considered);

(D) aerodynamic drag factor for a spherical body is taken to be 0.3 (according to different sources ranging from 0.1 to 0.4).

"Movement". The motion of drops in the atmosphere can be described by differential equations of free falling bodies in the air used in aerodynamics [5–7]. The mathematical package MathCAD was used for calculations.

The following system of differential equations used in the model:

$$\begin{cases} \frac{dh}{dt} = V \\ V' = -\frac{k1}{m} \cdot V^2 - \frac{k2}{m} \cdot V + g \end{cases}, \quad (1)$$

where h is the height where a drop begins to move, km; V is velocity of droplet, m s^{-1}; g is acceleration of gravity, 9.8 m s^{-2}; $k1$ is aerodynamic drag coefficient (the Stoke's formula); $k2$ is viscous friction; m is mass of the droplet, kg:

$$k1 = 6 \cdot \pi \cdot \mu \cdot r, \quad (2),$$

where μ is dynamic viscosity of the medium, for air at T = 14°C and P = 1 atm, μ = 17.7 × 10^{-3} N × C m^{-2}; r is droplet radius, m. Factor $k2$ is viscous friction:

$$k2 = \frac{1}{2} c \cdot S \cdot \rho_{medium}, \quad (3)$$

where c is drag index, relative units (for a sphere c = 0.3); S *is* cross-sectional area; ρ_{medium} *is* medium density, for air ρ_{air} = 1.29 kg m^{-3}.

Solution of differential equations of motion was carried out by numerical methods. According to the model, the following motion parameters of a drop were calculated:

• free-fall acceleration $a(t)$, m s^{-2};

• instantaneous drop velocity $V(t)$, m s^{-1};

• "terminal" velocity $V_c(h)$, m s^{-1};

• height over ground h, km;

• movement in a given height interval t, s.

Rain clouds are located at a height not more than 5 km from the earth's surface. Coincidently the bulk of pollution is concentrated at this altitude range. Therefore, the model calculation is made for the initial height of 5 km. The model allows making a calculation for any initial height.

Drop size for modeling is taken within a range of 1–6 mm, as the range of less than 0.5 mm belongs tosprays, drops larger than 6 mm are unstable and under the influence of gravity split at falling.

Free-fall acceleration in the initial phase at an altitude of 5 km (within 10–15 s) decreases up to 0. Schedule of acceleration is not given, since the rate schedule accurately reflects the acceleration. Speed of falling drops (size from 1 to 6 mm) at the initial phase at a height 5 km is shown in Fig. 1.

The diagram shows that the speed of falling rapidly reaches saturation. Gravity is balanced by the aerodynamic drag and viscous friction, the motion of the drop becomes steady. The set speed $V_c(h)$ is achieved in 10–15 sec.

Calculations of time required for reaching the set speed are shown in Fig. 2. The height at which the movement of a drop begins is laied off as abscissa. Thus, the falling drop reaches a steady speed at a distance of no more than 50 m.

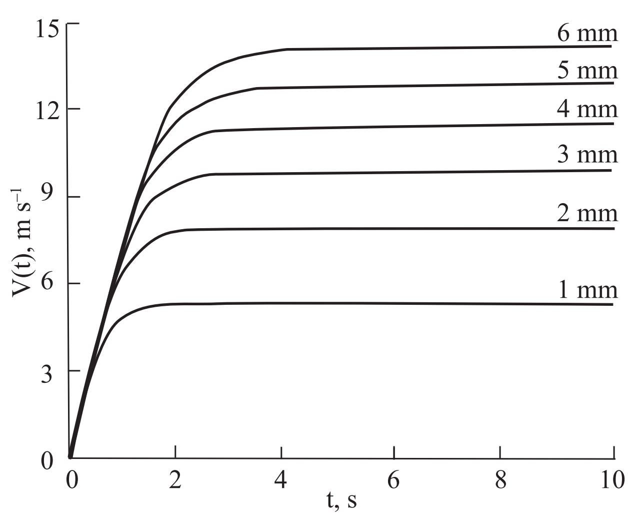

Fig. 1. Dropping speed at an altitude of 5 km at the initial phase of falling. Numerals at the curves correspond to the diameters of drops (d, mm). The same numerals are in Figs. 2, 3, 6 and 8.

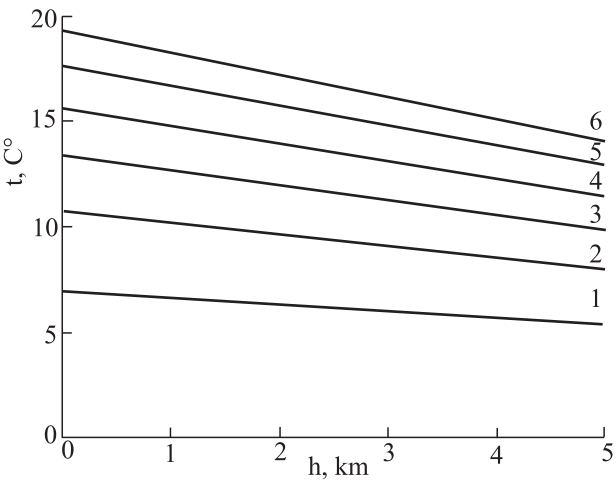

Fig. 2. Time dependence of achieving steady speed on the initial height of dropping.

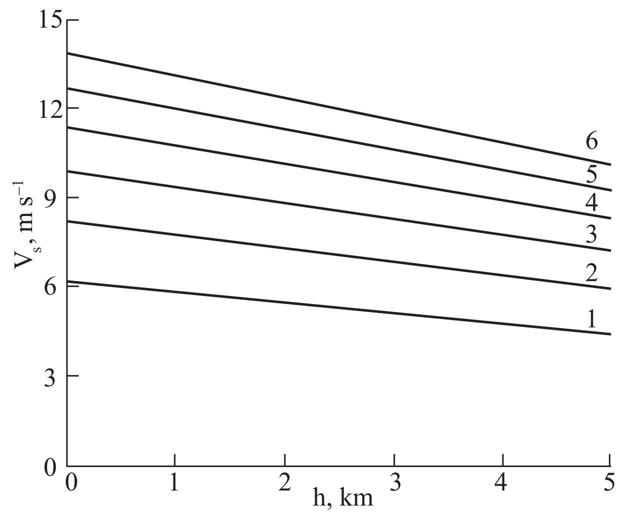

Fig. 3. Dependence of the steady dropping speed on height.

In most cases the initial section of a drop motion is above the pollution level, smog height is generally below cloud level, so the initial section of the movement is ignored. In this case the set speed can be calculated by the analytic dependence. Equating the acceleration to zero, the equation (1) can be solved as an ordinary quadratic equation. Then the set speed varies according to changes in air density:

$$V_c(h) = \frac{3\pi\mu d + \sqrt{9\pi^2\mu^2 d^2 + 2\,csR(h)mg}}{csR(h)} \tag{4}$$

$$R(h) = \rho_c \cdot exp(-\frac{h}{7.99}), \tag{5}$$

where $R(h)$ is air density at the altitude h, kg m^{-3}; h is the altitude, km; d is diameter of a drop, m; p_c is density of air at ground level, 1.293 kg m^{-3}. Dependence (5) is given in ref. [8].

The dependence of the set speed from the height for drops of six sizes is shown in Fig. 3. Starting point is 0 km, ground level is 5 km. At falling the set speed decreases due to the increasing density of the air and reaches 5–15 m s^{-1} at the ground level.

"The absorption of solids". To calculate the number of solids absorbed by drops, the following integral can be used:

$$F(t,i,d,D,H) = \int_5^0 \int_{d-\Delta}^{d+\Delta} \int_0^{20} \int_0^{t_1} N(D,H) \cdot Q(D,d) \cdot i \cdot f(d) \cdot dt \cdot dd \cdot dD \cdot dH, \tag{6}$$

where D is diameter of a solid (0–20) μm; d is droplet diameter (d–Δ — d+Δ), mm; I is rain intensity, mm h^{-1}, H is height (5–0), km; t is time, s; N (D, H) is the distribution of solids according to their size N (D, H) depending on their diameter and height above the ground; Q (D, d) is the efficiency of absorption of solids; i is rainfall intensity; f (d) is droplet size distribution.

Some simplifications been introduced, the equation is more convenient for calculation. Let's assume that:

• there is no droplet size distribution (Δ = 0);

• distribution of solids is constant at changing heights. In this case, the equation is as follows:

$$F(t,i,D,H) = H \cdot i \cdot t \int_0^{20} N(D) \cdot Q(D) dD \tag{7}$$

The calculation of the absorption of solids was carried out due to the method described in ref. [9]. The absorption coefficient is defined as:

$$N_I = \frac{V \cdot D^2 \cdot \rho_c}{18 \cdot \mu \cdot d}, \tag{8}$$

where V is velocity of a droplet, m s^{-1}.

The results of the absorption coefficient of solid particles, depending on the size of a drop for six solid particle sizes are shown in Fig. 4.

The dependence shows that the more absorption coefficient is, the smaller is the difference between the

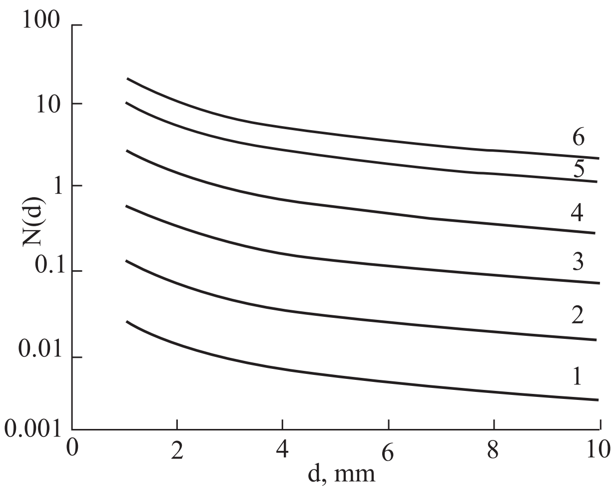

Fig. 4. Dependence of absorption coefficient of the solids for six particle sizes on the size of the drops. Numerals at the curves correspond to the diameters of particles (μm). The same numerals are in Fig. 5.

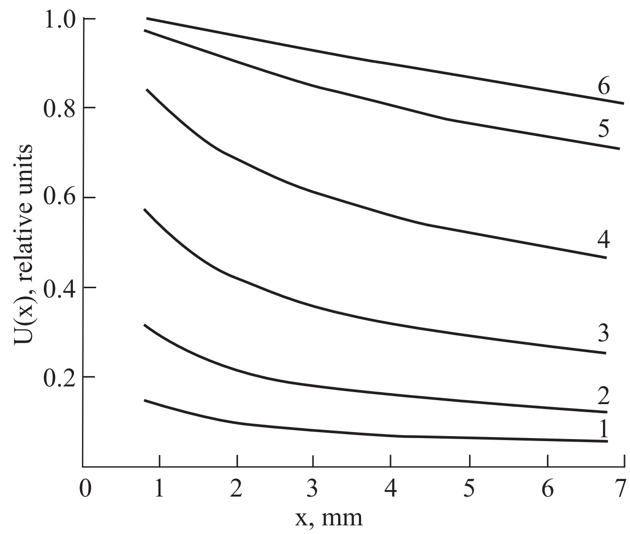

Fig. 5. Dependence of the trapping efficiency (relative units) on the size of a drop for six particle sizes.

droplet size and the size of the solids absorbed. If the difference between dimensions is great, for example, for diameter of 1 μm or less, the absorption coefficient decreases less than 0.01, indicating the absence of any absorption. Therefore, the particle size of less than 1 μm is not taken into account. Particles larger than 30 μm tend to precipitate independently and are also not considered.

The experimental dependence of the effectiveness of the inertial absorption of spherical particles is directly related to the absorption coefficient [9]. Dependence is well approximated by the following equation:

$$U(x) = 1 - \exp(-\sqrt{N_I}\,), \tag{9}$$

where x is particle diameter, μm; N_I is absorption criterion, relative units.

The results of calculating the efficiency of the inertial capture of particles ranging in size from 1 to 20 μm are shown in Fig. 5.

When the difference between the sizes of droplets and particles is more than 1000 times larger, the effectiveness of trapping the solids from the air and absorption, respectively, is practically equal to 0.

Distribution of dust-sized particles is described by equations (10 and 11) in ref. [9]:

$$y(D) := 3486\,\frac{1}{D^2} \tag{10}$$

$$F(D) = 3486 \cdot D^{-2} \tag{11}$$

Calculation of the total absorption of pollutant particles and the dynamics of air purification is performed on average values. Calculation of the average particle size is based on the average weight of a given concentration of particles. Hereafter, specific absorption of these particles over time and the percentage of air purification is calculated. The dependence of air purification (in %) on time is shown in Fig. 6 (rain of moderate intensity with an intensity 4 mm h^{-1}).

"Absorption of gaseous contaminants". To calculate the absorption of gaseous contaminants, firstly a drop at a steady state, i.e. resting, should be analyzed. In a steady state polluting substance being in a gaseous phase diffuses to the droplet surface. Adsorption of the pollutant takes place on the droplet surface. Then, the pollutant in the liquid phase diffuses into the drop. An equilibrium process is established, where the rate-limiting step determines the rate of transfer. In the near-surface zone of the gas phase the depleted zone appears, where the concentration of the contaminant decreases as it approaches the droplet surface.

In dynamic mode, i.e. during the drop falling, the near-surface zone updates continually, the multiplicity of air exchange is about 6 orders of magnitude. The velocity V of a drop with diameter 1 mm at a height 1 km is ~ 5 m s^{-1} (the rate of airflow $V \cdot \pi \cdot 2^{-1}$ is ~ 8 m s^{-1}). Average speed of molecules of SO_2 in the air is 100 m s^{-1} [8]. Multiplicity of air exchange K (K = h·d) within 1 km is 106. Molecules of the pollutant bombarding the surface are considered to be adsorbed on the surface of a drop with a coefficient of absorption A. Following is the calculation of the flow of the pollutant during a

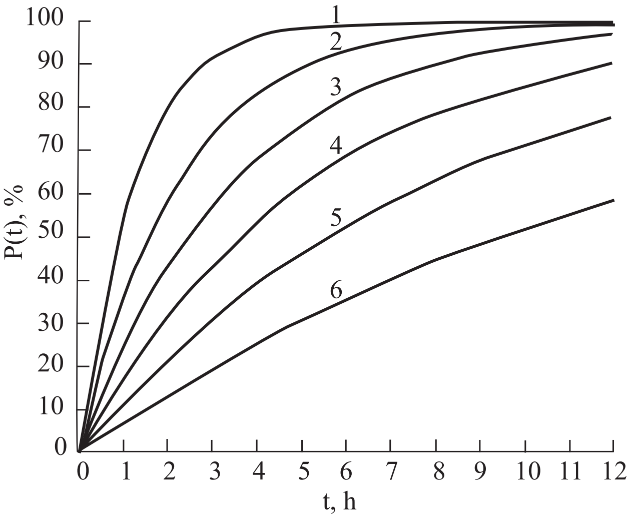

Fig. 6. The dynamics of air purification from contaminants by the rain of moderate intensity.

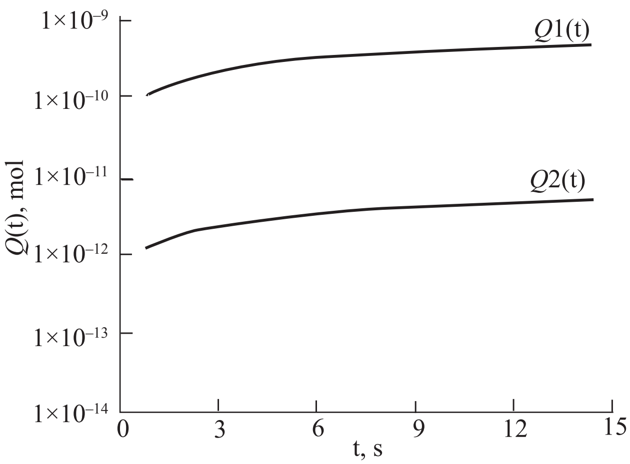

Fig. 7. Time dependence of the flow of a pollutant on the surface of a drop $Q1$, the flow of pollutant into a drop $Q2$.

single exchange cycle (i.e. time t = 1.25 × 10^{-4} s) for SO_2 by the diffusion mechanism. Pollutant flow $Q1$ on the droplet surface is:

$$Q1(\tau) = C_b \cdot A\sqrt{\pi D_1 \tau}\,, \qquad (12)$$

where C_b is concentration of pollutants in the air (for SO_2 C_b is 2 × 10^{-9} mol l^{-1}) [10]; D_1 is the diffusion coefficient of SO_2 in nitrogen (0.104 cm^2 s^{-1}) [11].

While accumulating molecules of a pollutant, the concentration on the surface will not exceed the maximum concentration C_p, which corresponds to the solubility of the substance in water R (for SO_2 C_p is 20.1 mol l^{-1}).

Accumulation of pollutants on the surface leads to simultaneous diffusion into the droplet. The flow of pollutant into a drop is also calculated by the diffusion mechanism:

$$Q2(\tau) = C_0 \cdot A\sqrt{\pi D_2 \tau}\,, \qquad (13)$$

where C_0 is surface concentration of a pollutant, mol l^{-1}; D_2 is the diffusion coefficient of SO_2 in water (1.4 × 10^{-5} cm^2 s).

Fig. 7 shows the time dependence of a pollutant flow on the surface of a drop and the flow of pollutant into a drop.

Obviously, the flow inside a drop is by two orders smaller than the flow at the droplet surface. Diffusion into a drop can be neglected. At detailed consideration these curves should be plotted as a function of height. In a first approximation, the dependence of pollutant concentration on the height is constant.

Number of pollutants captured by a falling drop from a height of 1 km is (QK$s1$) 4 × 10^{-10} mol ($s1$ = 3.14 × 10^{-4} dm^2).

Taking into account the decrease of a pollutant concentration in the air S_v for the rain of moderate intensity, the dynamic of air purification (decrease of pollutant concentration P (t), %) is shown in Fig. 8.

The air cleaning (in %) during 1 hour by the rain of moderate intensity is 78.8% for the diameter of droplets 1 mm, 17.2% for the diameter of drops 2 mm, 5.5%

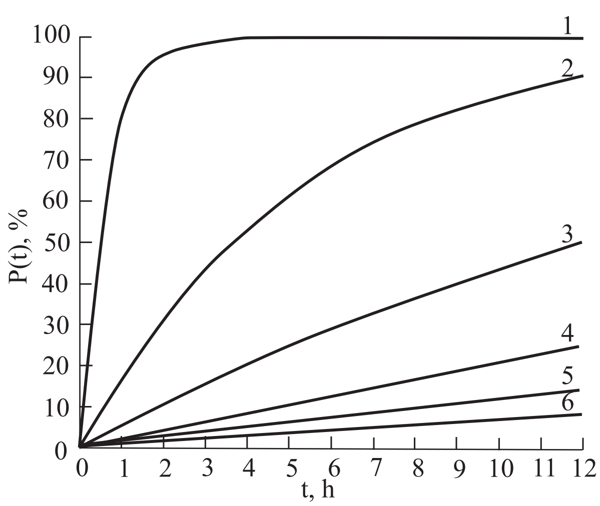

Fig. 8. The dynamics of air purification from SO_2 by the rain of moderate intensity.

for the diameter of drops 3 mm, 2.3% for the diameter of drops 4 mm, 1.2% for the diameter of drops 5 mm and 0.7% for the diameter of drops 6 mm. The Fig. 8 shows that the drops with smaller diameter purify the air more efficiently than the drops with larger diameter.

Thus, a mathematical model of air cleaning by rain is developed. The model allows to calculate the amount extracted solids and gaseous contaminants from the air depending on the time, rain intensity and droplet size. The concrete results of the calculations on the air cleaning from solids and sulfur dioxide are considered.

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