

Modeling the evolution of the aerosol cloud of toxicants in the atmosphere

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Abstract. Using the methods of mathematical modeling, the formation and evolution of aerosol clouds of toxicants in the atmosphere from the chemical industry enterprises, thermal power engineering and rocket carriers of space vehicles is analyzed. The processes of dynamic interaction of drops between themselves and a two-phase flow, processes of agglomeration, crushing and evaporation of aerosol particles are taken into account. The results of numerical calculations are presented.

1 Introduction

Increasing the impact of human life on the environment requires constant improvement of the means of monitoring this impact and analyzing its consequences. One of the most important objects of the described impact influence is the atmosphere. It accepts the toxicants flow ejected from the pipes of thermal power plants, chemical plants, etc. of. A significant contribution to the violation of the environment is made by space vehicles and aircraft, especially when forcibly dumping the remains of fuel components before a forced, unforeseen or emergency landing of the apparatus.

The present work is devoted to mathematical modeling of the formation, evolution and distribution of toxic aerosols in the atmosphere with the localization of the site of their deposition, the analysis of the possible degree of contamination for a particular area, taking into account various physical and meteorological factors in order to predict possible environmental risks. When formulating a mathematical model, the features of the processes of dynamic interaction of moving deformable particles (droplets) of a dispersed phase in the general case with a two-phase dispersion medium are considered [1-5]; the influence of meteorological features of the region is analyzed; the set of interrelated processes - deformation and fragmentation of drops with the analysis of processes of their evaporation and heat and mass exchange with a turbulent atmosphere [6-7] is taken into account. Reviews on this problem are presented in [8-9].

The paper presents the results of mathematical modeling of the evolution and dynamics of a liquid-drop cloud in the case of an emergency dump of liquid aviation or rocket fuel.

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2 Physical and mathematical models of processes

As shown by the analysis of the experimental data [10] in the range of moderate ($Re \approx 10 \div 100$) and small ($Re \leq 1$) Reynolds numbers in the region of large Bond numbers Bo typical for the aerosol droplets under consideration, the deformation of the droplet from the Weber number We [11] is determined by the relation:

$$\varepsilon = \frac{D_m}{D_0} = 1 + 0.027We, \quad (1)$$

where D_m is the diameter of the average cross section of the drop; D_0 - diameter of an equivalent spherical drop (whose volume is equal to the volume of the deformed drop).

The similarity criteria for the conditions of specific experiments using the following formulas were calculated:

$$Re = \frac{\rho |U - U_p| D}{\mu}, \quad We = \frac{\rho |U - U_p|^2 D}{\sigma}, \quad Bo = \frac{\rho_p D^2}{\sigma} |\omega|, \quad (2)$$

where σ is the coefficient of surface tension; ρ_p is the density of the drop.

The process of coagulation and fragmentation of aerosol particles on accordance with the generalized approximation formula for the collision parameter of droplets of a two-phase flow of similar sizes [11, 12] was modelled:

$$\Phi_{ji} = 1.4 + 1.979\beta + 0.507(2\beta^2 - 1), \quad (3)$$

$$\text{where } \beta = \left(\frac{Re_{ji}}{383.6} \right)^{0.572} \left(\frac{Lp_i}{370.37} \right)^{-0.153} \left(\frac{\gamma_{ji}}{2.37} \right)^{-0.597}; \quad \Phi_{ji} \text{ is the mathematical expectation}$$

of the ratio of the change in the mass of the target drop D_i , caused by the interaction of $j-i$, to the total mass of the projectile droplets D_j ($D_j < D_i$) that collide with it. $Re_{ji} = 6$ to 385; $Lp_i = 0.2$ to 600; $Re_{ji} = 1 \div 12$; Re_{ji} - Reynolds number, calculated by the diameter of the drop-projectile D_j ; Lp is the Laplace number; γ_{ji} is the ratio of the diameters of the colliding drops.

The Reynolds number from the diameter of the D_j projectile was calculated. Equations of motion of a droplet of radius r_p for the its velocity componens in a Cartesian coordinate system relative to the surface (the z axis is directed along the gravitational acceleration vector of gravity) has the form [11]:

$$\frac{du_p}{dt} = \varphi_1(u - u_p), \quad \frac{dv_p}{dt} = \varphi_1(v - v_p), \quad \frac{dw_p}{dt} = \varphi_1(w - w_p) + g, \quad (4)$$

$$\text{where } \varphi_1 = \frac{3\rho}{8\rho_p r_p} C_D |U - U_p|; \quad |U - U_p| = \sqrt{(u - u_p)^2 + (v - v_p)^2 + (w - w_p)^2}; \quad u, v, w$$

are the components of the wind speed vector U ; u_p, v_p, w_p are the components of the velocity vector of the droplet U_p ; C_D is the coefficient of aerodynamic resistance.

At $Re = (1 \div 700)$ (intermediate flow regime), the Klyachko formula to determine the coefficient of aerodynamic drag was used [13]:

$$C_D = \frac{24}{Re} + \frac{4}{\sqrt[3]{Re}}. \tag{5}$$

For $Re = (700 \div 3 \cdot 10^5)$ (self-similar flow) [14], $C_D = 0.44$ was assumed. The process of aerodynamic crushing of droplets was determined in accordance with the calculated values of the Weber and Bond criteria. In accordance with the analysis of the experimental data, it was assumed that when the critical Weber number $We=We^*=17$ or the critical value of the Bond number is $Bo=Bo^*=22.5$, the drop is split into two spherical drops of equal mass. The physical properties of air due to vertical coordinate of account for a specific date using the parameters of the standard atmosphere and the data of weather stations was taken on. The coefficient of dynamic viscosity of air using the Sutherland formula [15] was calculated:

$$\mu = \frac{0.68 \cdot 10^{-2}}{T + 122} \left(\frac{T}{273} \right)^{3/2},$$

where T is the absolute temperature.

The drop is a thermally thin body, and its temperature averaged over the volume T_p in accordance with the following equation was determined:

$$\frac{dT_p}{dt} = \varphi_2 Nu(T - T_p) - \frac{q_r}{mc_p} G, \tag{6}$$

where $\varphi_2 = \frac{3}{2} \frac{\lambda}{r_p^2 \rho_p c_p}$; c_p is the specific heat of the liquid; λ is the coefficient of thermal

conductivity of air; m is the mass of the drop; G is the mass of the evaporated liquid from the drop surface per unit time (evaporation rate); q_r is the specific heat of evaporation of the liquid.

To calculate the Nusselt number, the following dependence was used [16]: $Nu=2+0.6Re^{1/2}Pr^{1/3}$, where Pr is the Prandtl number. The change in the droplet radius due to evaporation on the equation was determined:

$$\frac{dr_p}{dt} = - \frac{G}{4\pi\rho_p r_p^2} \tag{7}$$

The evaporation rate by the formula was determined:

$$G = 4\pi r_p^2 k \frac{X}{1-X}, \tag{8}$$

where k is the mass-transfer coefficient; X is the mole fraction of the vapor near the drop surface.

Equation (7) in accordance with the relationship between X and the partial vapor pressure p_0 was written:

$$\frac{dr_p}{dt} = - \frac{k}{\rho_p} \frac{p_0}{p - p_0}, \tag{9}$$

where p is the atmospheric pressure. The mass-transfer coefficient k from the formula [17] was calculated:

$$k = \frac{c_f D_f M_p}{2r_p} \left[2 + 0.6 \left(\frac{2r_p |\mathbf{U} - \mathbf{U}_p| \rho_f}{\mu_f} \right)^{1/2} \left(\frac{\mu_f}{\rho_f D_f} \right)^{1/3} \right], \quad (10)$$

where D_f is the binary diffusion coefficient at the film temperature $T_f = (T_f + T)/2$; c_f and μ_f are the density and coefficient of dynamic viscosity of air at T_f .

The diffusion coefficient in accordance with the Fuller-Schletter-Giddings [18] proposals for binary gas systems at low pressure was calculated:

$$D = \frac{T^{1.75} [(M_A + M_B) / (M_A M_B)]^{0.5}}{p \left[(\sum V_A)^{1/3} + (\sum V_B)^{1/3} \right]^2}, \quad (11)$$

where $[D_f] = \text{cm}^2/\text{sec}$; $[p] = \text{atm}$; $[T] = \text{K}$; M_A and M_B are the molecular masses of components A and B (drops of liquid and air); $\sum V_A$, $\sum V_B$ are the diffusion volumes of molecules.

The trajectory of droplet motion was determined in accordance with kinematic equations:

$$u_p = \frac{dx}{dt}, v_p = \frac{dy}{dt}, w_p = \frac{dz}{dt}. \quad (12)$$

3 Simulation results

For numerical integration of the system (4) - (12), the implicit difference scheme for the linearized right-hand sides was used [11]. In the calculations, the dynamics of each droplet fraction with a fixed size in the range 0-3 mm was separately analysed. At each time step, the kinematics of the motion is separately considered, taking into account the possibility of aerodynamic fragmentation of the droplet, the new droplet coordinates and the components of its velocity vector are determined, the new droplet temperature is determined, and finally, the droplet size are modelled taking into account evaporation. Integration of the system of equations for each fraction until the droplet evaporates completely or when it reaches, the surface of the Earth is carried out. The reliability of the results of numerical modelling of the formation and the dynamics of the change in aerosol clouds of toxicants in the atmosphere comparison with typical experimental data of the results of the launch of the "Proton" carrier rocket on October 26, 2007 [10] was verified by. In this case, the toxicant was an asymmetric dimethyl hydrazine (component of liquid fuel), and the height of the formation of the toxic aerosol cloud was about 30 103 m. The projections of the trajectories of aerosol particles of the main calculated fractions shows in Fig. 1. The experimentally confirmed discrepancy between the trajectories of different particle sizes the influence of the wind speed varying in altitude was explained by.

The change in the rate of evaporation of particles in height corresponds due to the change of the atmospheric temperature on altitud (Fig. 2).

Figure 2 shows the rate of evaporation G in height, defined as the mass of evaporated toxicant per meter of fall height and the corresponding atmospheric temperature t . Completely evaporation of drops of a maximum initial size of 3 mm took place at an altitude of 2200 m. Good qualitative and satisfactory quantitative coincidence of the calculations and analysis contained in [10] allows us to recommend the calculation methodology developed by the authors for its use in assessing the impact of thermal energy facilities, chemical plants, etc. on the environment.

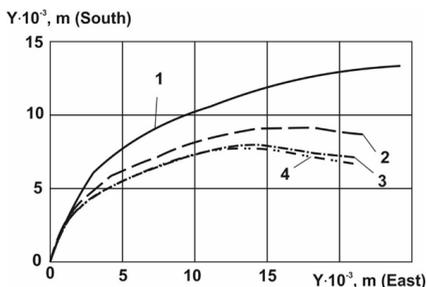


Fig. 1. Projections of trajectories of particles of different initial radius on a horizontal plane. 2 mm - curve number 1; 3 mm - curve number 2; 1.5 - curve number 3; 1 mm - curve number 4.

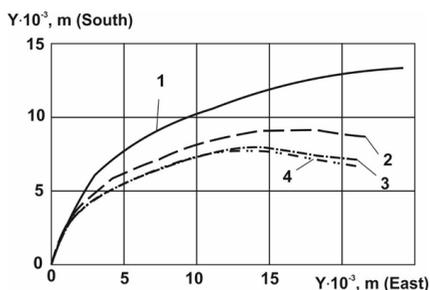


Fig. 2. Mass evaporation rate G and temperature of the atmosphere t in height.

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