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Modeling the spread of aerosol cloud into the atmosphere

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Abstract

A physical-mathematical model for describing the propagation of liquid-droplet components of the rocket propellant in areas of falling the launcher separated units is presented. The results of calculation of the unsymmetrical dimethylhydrazine droplet cloud evolution, formed at the second stage of «Proton-K» launcher separation above the Tomsk Region at starts from Baikonur Cosmodrome (Russia) are analyzed.

Keywords: Ecology; atmosphere, boosters; liquid propellant; toxic components; liquid-drop cloud evolution; complex approach; mathematical modeling.

At the stage separation of liquid-propellant carrier rockets may result in atmospheric emissions of the toxic propellant components. The emission of these components is accompanied by a set of complex interrelated physicochemical processes (evaporation, chemical heterogeneous reactions, diffusion, coagulation, splitting of droplets, etc. To assess ecological consequences of such events and the damage to the target territories, it is necessary to have reliable physicochemical models of the considered processes. When constructing the physicochemical model of a spread of liquid- droplet toxic components, it is necessary to understand the following processes in detail:

- the formation of the primary droplet cloud at the time of depressurization of fuel tanks;
- processes of droplet evaporation at a sharp change of the ambient conditions due to depressurization;
- diffusion and spread of the components under the action of the dominant wind;

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- chemical reactions of the propellant components with the atmosphere;
- processes of gravitational sedimentation of droplets with the allowance for evaporation and splitting upon interaction with gas, as well as the gravitational coagulation and splitting upon mutual collision of different-size droplets.

In this paper we describe a physical-mathematical model of propagation of a cloud of propellant liquid droplets in the atmosphere (Arkhipov et al., 2004; Adam et al., 2007).

The equation of a moving droplet with r_p radius in the projection on the axis of rectangular coordinate system x , y , z (the axis z is directed along the vector of the acceleration do to the gravity \mathbf{g} of free fall) have the form (Vasenin et al., 1986):

$$\frac{du_p}{dt} = \phi_1(u - u_p), \quad \frac{dv_p}{dt} = \phi_1(v - v_p), \quad \frac{dw_p}{dt} = \phi_1(w - w_p) + g \quad (1)$$

where: $\phi_1 = \frac{3\rho}{8\rho_p r_p} C_D |\mathbf{v} - \mathbf{v}_p|$; $|\mathbf{v} - \mathbf{v}_p| = \sqrt{(u - u_p)^2 + (v - v_p)^2 + (w - w_p)^2}$

u , v , w are components of the wind speed vector \mathbf{v} ; u_p , v_p , w_p are components of the droplet speed vector \mathbf{v}_p ; ρ is the air density; ρ_p is the liquid density; C_D is the aerodynamic drag coefficient.

To estimate the aerodynamic drag coefficient the Klyachko formula (Klyachko, 1934) was used:

$$C_D = \frac{24}{\text{Re}} + \frac{4}{\sqrt[3]{\text{Re}}} \quad (2)$$

where $\text{Re} = 2\rho |\mathbf{v} - \mathbf{v}_p| r_p / \mu$ is the Reynolds number of the relative motion; μ is the coefficient of the air dynamic viscosity.

The dependence (2) is true within $\text{Re} = (1 \div 700)$ (intermediate flow mode). $C_D = 0.44$ was used at $\text{Re} = (700 \div 3 \cdot 10^5)$ (self-similar flow mode) (Vasenin et al., 1986).

To take into account the aerodynamic droplet splitting, the Weber and Bond criteria were calculated:

$$\text{We} = \rho |\mathbf{v} - \mathbf{v}_p|^2 D / \sigma \quad \text{Bo} = 4\rho_p |\mathbf{a}| r_p^2 / \sigma$$

where σ is the liquid surface tension coefficient; \mathbf{a} is the droplet acceleration vector.

It was assumed that on reaching the critical value of Weber number $\text{We} = \text{We}^* = 17$ or critical value of Bond number $\text{Bo} = \text{Bo}^* = 22.5$, the droplet splits into two spherical droplets of equal masses.

Accounting for the influence of vertical coordinate on air physical properties was made for a particular launch date using parameters of the standard atmosphere and weather station data. The coefficient of the air dynamic viscosity was calculated by the Sutherland's formula (Abramovich, 1991):

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

where T is the air absolute temperature.

Since droplet move in different atmospheric layers, their heat exchange with the environment takes place. Therefore, the temperature of a droplet T_p was calculated by following heat balance equation:

$$\frac{dT_p}{dt} = \phi_2 \text{Nu} (T - T_p) - \frac{q_{vap}}{mc_p} G \quad (3)$$

$$\text{where } \phi_2 = \frac{3}{2} \frac{\lambda}{r_p^2 \rho_p c_p} ;$$

c_p is the specific heat capacity of liquid; λ is the coefficient of the gas thermal conductivity; T_p is the droplet temperature (averaged over volume); m is the droplet mass; G is the liquid mass evaporating from the droplet surface per unit time (evaporation rate); q_{vap} is the specific heat of the liquid evaporation.

To calculate the Nusselt number, we used the following dependence (Aggorvol et al., 1985): $Nu = 2 + 0.6Re^{1/2}Pr^{1/3}$ where Pr is the Prandtl number.

The equation for variation of the droplet radius due to evaporation has the form:

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

Evaporation rate is determined by the following formula:

$$G = 4\pi r_p^2 k \frac{X}{1-X} \tag{5}$$

where k is the coefficient of the mass transfer; X is mole fraction of the droplet matter vapor near its surface.

Having expressed X through the vapor partial pressure p_0 , we can write equation (4) in the following form:

$$\frac{dr_p}{dt} = - \frac{k}{\rho_p} \frac{p_0}{p - p_0} \tag{6}$$

where p is the pressure of the ambient medium.

The coefficient of mass transfer k is calculated by the formula (Berd et al., 1974):

$$k = \frac{c_f D_f M_p}{2r_p} \left[2 + 0.6 \left(\frac{2r_p |\mathbf{v} - \mathbf{v}_p| \rho_f}{\mu_f} \right)^{1/2} \left(\frac{\mu_f}{\rho_f D_f} \right)^{1/3} \right] \tag{7}$$

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

The coefficient of dynamic diffusion for gas systems at low pressure was calculated by the Fullers–Shletter–Giddings method (Rid et al., 1982):

$$D = \frac{T^{1.75} [(M_A + M_B) / (M_A M_B)]^{0.5}}{p \left[(\sum V_A)^{1/3} + (\sum V_B)^{1/3} \right]^2} \tag{8}$$

where $[Df] = \text{cm}^2/\text{sec}$; $[p] = \text{atm}$; $[T] = \text{K}$; M_A and M_B are the molecular masses of A and B (liquid droplets and air); $\sum V_A$, $\sum V_B$ are the molecular diffusion volumes. The values of molecules diffusion volume for different substances are listed in (Bird et al., 1974). Formulae for calculation of the coefficient of diffusion in air of unsymmetrical dimethylhydrazine (UDMH) droplets were obtained with the help of equation (8):

$$D_f = \frac{0.9}{p} \left(\frac{T_f}{273} \right)^{1.75} .$$

To calculate the trajectories of droplet movement, the system of equations should be supplied with kinematic relations:

$D_f = \frac{T^{1.75} [(M_A + M_B) / (M_A M_B)]^{0.5}}{p \left[(\sum V_A)^{1/3} + (\sum V_B)^{1/3} \right]^2} \tag{9}$	(9)
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The system (1)–(9) is integrated numerically after substituting into it of values of wind speed components u , v , and w . The efficient implicit difference scheme (Vasenin et al., 1986) was used in the integration.

Initial conditions include droplet distribution according to their sizes, the initial cloud dimension, initial speed of droplets, depressurization altitude, droplet concentration, as well as the database of atmosphere parameters and wind speed at different altitudes. The main physical-chemical characteristics of UDMH (Sarner, 1969; Aleksandrov, 1993) are presented in Table ($T_r = T_p/T_c$ is the reduced film temperature).

Table. The main physical characteristics of UDMH ($\text{CH}_3)_2\text{NNH}_2$.

Characteristic	Symbol	Value
Molecular weight	M	60.102
Melting temperature	T_{melt}	-57.2 °C
Boiling temperature	T_{boil}	63.1 °C
Critical temperature	T_c	250 °C
Surface tension coefficient	σ	$5.88 \cdot 10^{-2} - 1.157 \cdot 10^{-4} T$, N/m
Density	ρ_p	$[810 - (T_p - 273)]$, kg/m ³
Evaporation heat	q_{vap}	$RT_c[7.08(1 - T_r)^{0.354} + 4.1172(1 - T_r)^{0.436}]$, J/kg
Gas constant of vapors	R	138.339 J/(kg·K)
Density of UDMH saturated vapor	ρ_{vap}	$\frac{0.9643}{T} \exp\left(\frac{16.78T - 3745}{T - 52.27}\right)$, kg/m

Fig. 1 presents the calculations results for actual «Proton-K» launch on October 26, 2007. The data for 12.00 GST on the day of start were used. Remote sensing data were obtained only for the altitude up to 23.6 km. The actual altitude of depressurization was 25÷35 km. We conducted parametric calculations for different UDMH droplet sizes, emission altitude (fuel tank depressurization) for actual weather conditions. Actual aeroclimatic data for the dates of «Proton-K» launches were obtained from Kolpashevo weather station database. As is seen, droplets of different sizes have evaporated at altitudes between 2.3 and 5.5 km.

The calculations presented in Fig. 2 refer to the actual start of «Proton-K» on December 26, 2007. This day was characterized by sharp changes of atmospheric conditions (temperature decrease, change of wind force and direction). Therefore, the calculations were conducted for three different time intervals supplied with remote sensing data: 00:00 and 12:00 GST on December 25, as well as 00:00 GST on December 26. The expected regions of UDMH droplets fallout for these time intervals are denoted in Fig. 4 by curves 1, 2, and 3. As is seen, the fall areas of UDMH droplets are mostly determined by the wind force and direction. The spread is quite wide. The actual fall area (the time of the stage depressurization is ~00:00 of Moscow time on December 27) can be found with the help of time interpolation between regions 2 and 3.

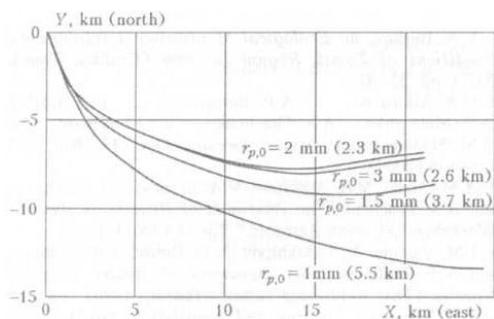


Fig. 1. The projection of trajectories of particles with different initial radii $r_{p,0}$ on the horizontal plane (the altitude of complete evaporation is given in brackets).

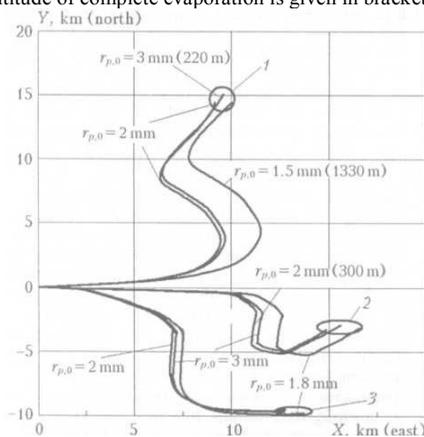


Fig. 2. The projection of trajectories of particles with different initial radii $r_{p,0}$ on horizontal plane (the altitude of complete evaporation is given in brackets).

In contrast to the October start, in December droplets of some sizes reached the surface, which is explained by a lower temperature in December as compared to October both in upper atmospheric layers and in troposphere.

The level of atmosphere temperature in its turn determines heptil droplets evaporation rate. Fig. 3 presents the evaporation rate of UDMH droplets with 3 mm initial radius at different altitudes. The abscissa axis denotes the evaporation rate (kg/m), i.e., the quantity of UDMH entering the atmosphere in the form of vapor per altitude unit. This parameter characterizes the level of atmospheric pollution at different altitudes, being convenient to solve numerous ecological problems. In practice, at high altitudes the droplets instantly freeze and do not evaporate. During the October start, at an altitude of 12.5–15 km the air temperature rises higher than UDMH melting temperature ($-57.2\text{ }^{\circ}\text{C}$), and the process of evaporation starts. Then the temperature again falls and the secondary evaporation begins at altitudes lower than 10 km. The droplets of a given initial radius (3 mm) are completely evaporated at an altitude of 2.2 km. In December, the evaporation process starts only at an altitude of 7.5 km due to lower temperatures, therefore, droplets of the above size cannot be evaporated completely and fall at the ground surface.

Thus the calculations have shown that in October the droplets of all dimensions evaporated at altitudes from 2.3 to 5.5 km and in December the intensive evaporation process starts only at much lower altitudes due to lower temperatures; there is not enough time for the droplets of some sizes to evaporate completely, therefore, they fall on the surface. In this case the contamination of the area is possible. As the calculations show, the

troposphere temperature profile (lower than 10 km) is the determining factor. Besides, we have revealed a significant influence of actual weather conditions at the moment of the launcher stage depressurization on the location of the cloud fallout area. The developed model can be used for solution of a great number of problems connected with the distribution of aerosol systems.

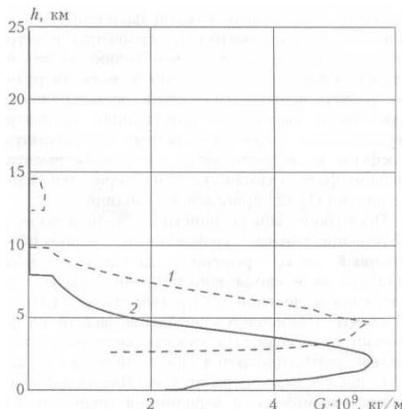


Fig. 3. UDMH droplets evaporation rate at different altitudes: October 26 (1); 00:00 GST on December 26, 2007 (2).

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