

Influence of weather conditions on the spread of aerosol cloud of liquid propellant

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Received February 13, 2008

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 model was developed with accounting for the real weather conditions. The results of calculation of the asymmetrical dimethylhydrazine droplet cloud evolution, formed at the second stage of "Proton-K" launcher separation above the Tomsk Region at starts from Baikonur Cosmodrome on October 26 and December 26, 2007, are analyzed.

Since 1967, the territory of Tomsk Region is used for dislocation of fall areas for launcher separated units (LSU), which start from Baikonur Cosmodrome.¹ The total area of 13 fall districts is equal to 2.14 mln hectares (Fig. 1). Since 1967, there were more than 260 starts of rockets, the LSU of

which fell on these areas: "Soyuz," "Zenith," "Proton," "Cyclone," and intercontinental ballistic missiles. Five starts were in 2006, one of which was "Proton-K" (Fig. 2). A very toxic unsymmetrical dimethylhydrazine (UDMH) also known as "heptil" was one of the components of this rocket propellant.

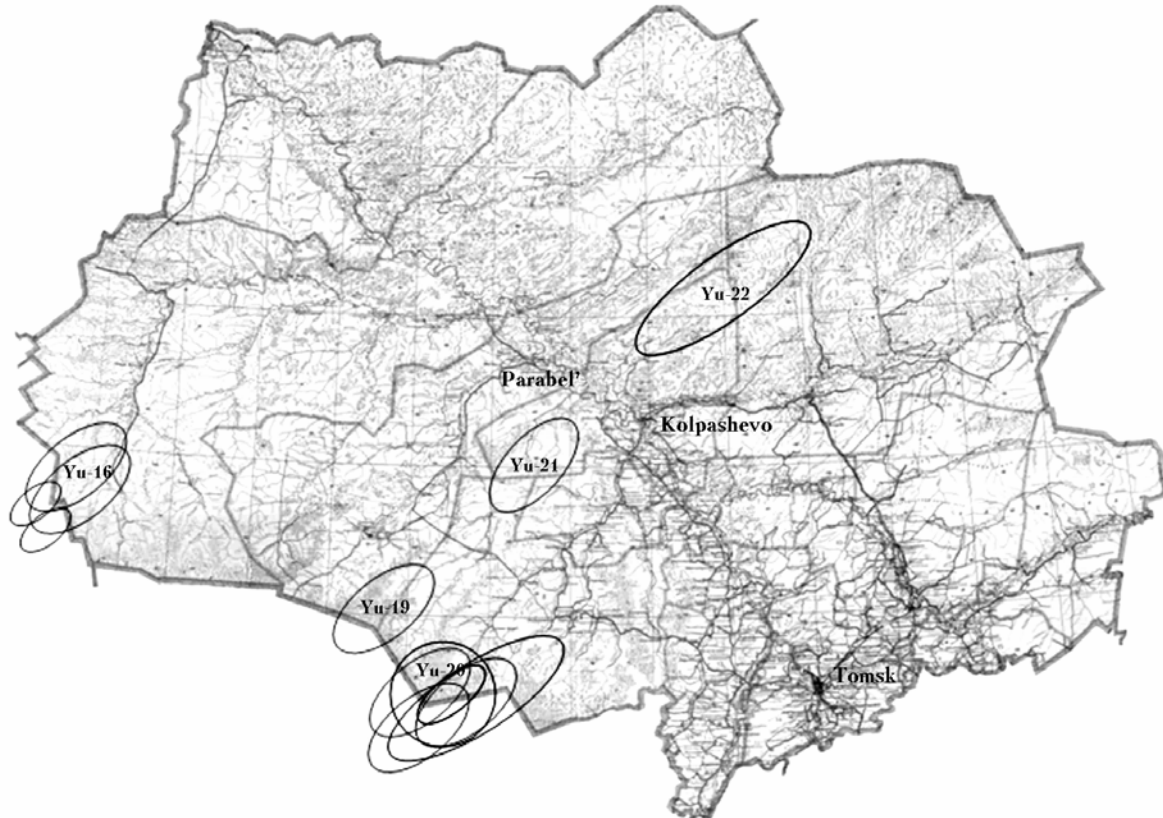


Fig. 1. Areas of LSU falls at the Tomsk Region.

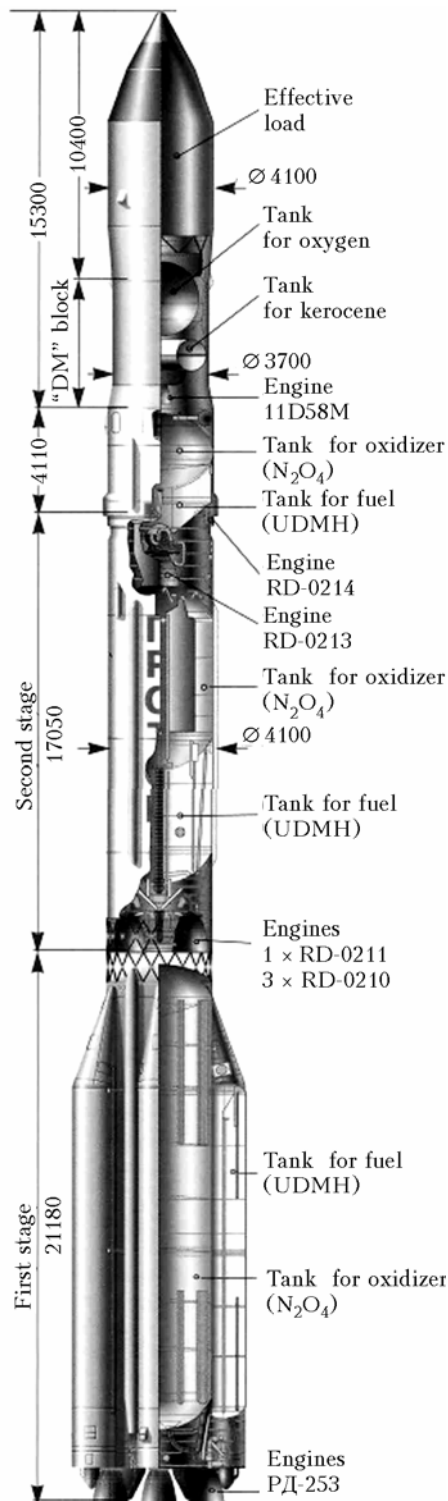


Fig. 2. "Proton-K" launcher.

The second stage of the launcher falls on Yu-21 area (see Fig. 1). This stage has the following characteristics:

- propellant components:
 - oxidizer – nitrogenous tetroxide;
 - fuel – unsymmetrical dimethylhydrazine;

- the weight of the stage with full tank is equal to 167.92 t;
- dry weight is equal to 11,75 t;
- length is 17,05 m;
- maximal lateral dimension is 4.1 m;
- engine operating period is 230 sec.

Having worked, the second stage of "Proton-K" launcher, having the velocity of 4.3 km/s, separates in 337 s after the start at an altitude of 155 km and 590 km away from the start point. After its separation the stage continues to move along the ballistic trajectory. Having flown 1200 km in the airless space, it enters atmospheric dense layers at a velocity of 4.5 km/s.

During its descent into dense layers the second stage undergoes a heavy aerodynamic loading. The temperature of the stage elements rises up to 1100°C and the stage breaks into fragments at the altitude of 25–35 km. The components of the propellant in tanks (reserve supply) and in trunk lines partially burn out mixing with each other and the air flow. The unburned fuel can evaporate, condensate, disperse, and finally fall on the ground.

The results of investigation conducted in "Oblkompriroda" laboratory and "ECO-Vector" laboratory (Novosibirsk) at the Yu-21 area of "Proton-K" LSU fall during the starts of 2006 has shown the absence of heptil in snow samples (more than 20 samples were taken). At the same time there is a probability that aerosol cloud of toxic components in the course of its evolution can fall in remote regions under action of turbulent diffusion and wind. Taking into account a high toxicity of UDMH and its long-term effect, it is important to define possible polluted regions. This can be done only with the help of numerical simulation using physical-mathematical models, adequately describing all physical factors, processes, and phenomena, which accompany the aerosol cloud propagation.

In this paper we describe a physical-mathematical model of propagation of a cloud of propellant liquid droplets in the atmosphere,^{2,3} taking into account actual weather conditions, including the air temperature, as well as the wind direction and speed at different altitudes. Each cloud droplet emitted at a certain initial speed and temperature is affected during its movement in the atmosphere by the gravity force directed downward, Archimedean buoyancy force directed upward, and the force of aerodynamic drag. The temperature of a droplet changes with time due to the process of heat-exchange. Besides, the droplet evaporates, decreasing in size. The evaporation process also makes its contribution to the heat-exchange. Therefore, the equation of droplet movement should be supplemented by the equation of heat-exchange and the equation of the droplet size change at the expense of its evaporation.

In the simulation, Archimedean buoyancy force is neglected because of its smallness. Thus, the equation of a moving droplet with r_p radius in the

projection on the axis of rectangular coordinate system x, y, z (z axis is directed towards the direction of the acceleration vector \mathbf{g} of free fall) has the following form⁴:

$$\begin{aligned}\frac{du_p}{dt} &= \varphi_1(u - u_p), \\ \frac{dv_p}{dt} &= \varphi_1(v - v_p), \\ \frac{dw_p}{dt} &= \varphi_1(w - w_p) + g.\end{aligned}\quad (1)$$

Here

$$\varphi_1 = \frac{3\rho}{8\rho_p r_p} C_D |\mathbf{v} - \mathbf{v}_p|;$$

$$|\mathbf{v} - \mathbf{v}_p| = \sqrt{(u - u_p)^2 + (v - v_p)^2 + (w - w_p)^2};$$

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 formula⁵ was used:

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

where $\text{Re} = \frac{2\rho|\mathbf{v} - \mathbf{v}_p|r_p}{\mu}$ is the Reynolds number of the relative movement; μ is the coefficient of dynamical water 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).⁴

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

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

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 atmosphere⁶ and weather station data. The dynamic viscosity coefficient was calculated by the Sutherland's formula⁷:

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

where T is the absolute air temperature; $[\mu] = \text{Pa} \cdot \text{sec}$. The error in calculating μ by this formula does not exceed 0.5% in temperature range 180–1400 K.

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

$$\frac{dT_p}{dt} = \varphi_2 \text{Nu}(T - T_p) - q_{\text{evap}} \frac{G}{m c_p}, \quad (3)$$

where

$$\varphi_2 = \frac{3}{2} \frac{\lambda}{r_p^2 \rho_p c_p};$$

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_{evap} is the specific heat of the liquid evaporation.

To calculate the Nusselt number, we used the following dependence⁸:

$$\text{Nu} = 2 + 0.6 \text{Re}^{1/2} \text{Pr}^{1/3},$$

where Pr is the Prandtl number.

The equation for a change of droplet radius due to evaporation has the following form

$$\frac{dr_p}{dt} = - \frac{G}{4\pi\rho_p r_p^2}. \quad (4)$$

Evaporation rate is determined by the following formula

$$G = 4\pi r_p^2 k \frac{X}{1 - X}, \quad (5)$$

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

$$\frac{dr_p}{dt} = - \frac{k}{\rho_p} \frac{p_0}{p - p_0}, \quad (6)$$

where p is the pressure of the ambient medium.

The coefficient of mass transfer is calculated by the formula⁹:

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

where D_f is the coefficient of binary diffusion at the film temperature $T_f = (T_p + T)/2$; c_f is the

summarized (air and UDMH vapor) volume mole concentration at T_f ; ρ_f is the summarized density of air and UDMH vapor mixture; μ_f is the dynamic air viscosity coefficient at T_f .

There exist a lot of methods for calculation of diffusion coefficient in binary gas systems at low pressure,⁹ however, the Fullers–Shletter–Giddings method is the most accurate among them, because it is based on a great body of experimental data.¹⁰ The empiric correlation has the following form

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

where $[D] = \text{cm}^2/\text{sec}$; $[p] = \text{atm}$; $[T] = \text{K}$; 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 Ref. 9. Formulae for calculation of the coefficient of diffusion in air of UDMH droplets were obtained with the help of equation (8):

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

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

$$\frac{dx}{dt} = u_p, \quad \frac{dy}{dt} = v_p, \quad \frac{dz}{dt} = w_p. \quad (9)$$

This system is integrated numerically after substituting into it of values of wind speed components u , v , and w . The efficient implicit difference scheme⁴ was used in the integration.

The system of equations (1)–(8) describes the movement of centers of mass of droplets for each fraction, taking into account evaporation, aerodynamic subdivision, and wind drift. In order to solve this system, we have to set initial conditions (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 [Refs. 11, 12] are presented in Table.

Since the task is described by nonlinear differential equation, we use numerical method for its solution. Differential equations are substituted by finite-difference equation with the use of difference scheme, implicit for right-side members. The task is divided into physical processes. Three physical processes separately are considered at each time step. At the first step, the movement equations are solved,

taking into account the possibility of droplet aerodynamic splitting as soon as critical values of Bonds or Webers numbers are reached, which allow setting of new droplet coordinates, as well as the components of its velocity vector. At the second step, the heat exchange equation is integrated and the droplet new temperature is determined. At the third step the change of the droplet radius and mass due to the evaporation process is found. These calculations continue until the vertical coordinate of the droplet coincides with the Earth surface or the droplet completely evaporates.

Table. The main physical characteristics of UDMH (CH₃)₂NNH₂

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_{evap}	$RT_c[7.08(1 - T_r)^{0.354} + 4.1172(1 - T_r)^{0.456}]$, J/kg
Gas constant of vapors	R	138.339 J/(kg·K)
Density of UDMH saturated vapor	ρ_n	$\frac{0.9643}{T} \exp\left(\frac{16.78T - 3745}{T - 52.27}\right)$, kg/m ³

Note. T_r is the reduced film temperature: $T_r = T_f/T_c$. The temperature is taken in K in the approximation formulae.

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.

Figure 3 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. As is seen, droplets of different sizes have evaporated at altitudes between 2.3 and 5.5 km.

The calculations presented in Fig. 4 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 figures 1, 2, and 3.

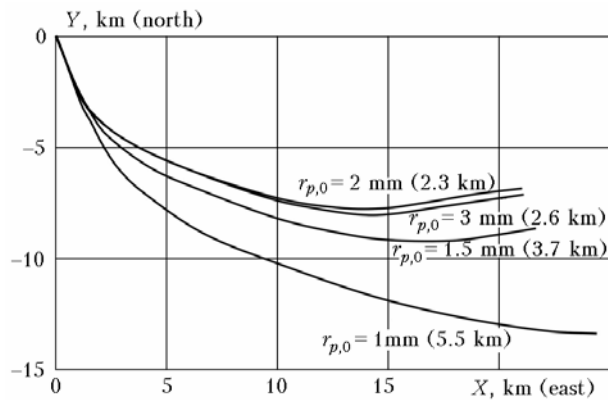


Fig. 3. The projection of trajectories of particles with different initial radii $r_{p,0}$ on the horizontal plane for “Proton-K” on October 26, 2007 (the altitude of complete evaporation is given in brackets).

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 approximately 00:00 of Moscow time on December 27) can be found with the help of time interpolation between regions 2 and 3 (see Fig.4).

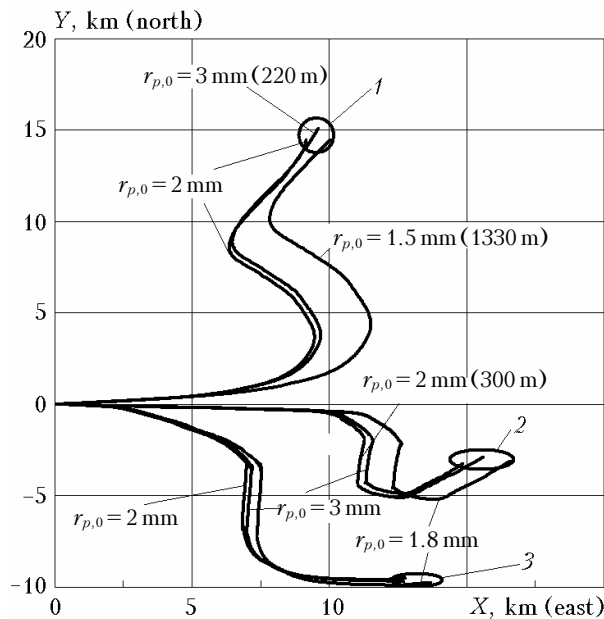


Fig. 4. The projection of trajectories of particles with different initial radii $r_{p,0}$ on horizontal plane for “Proton-K” on December 26, 2007 (the altitude of complete evaporation is given in brackets).

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 (Fig. 5).

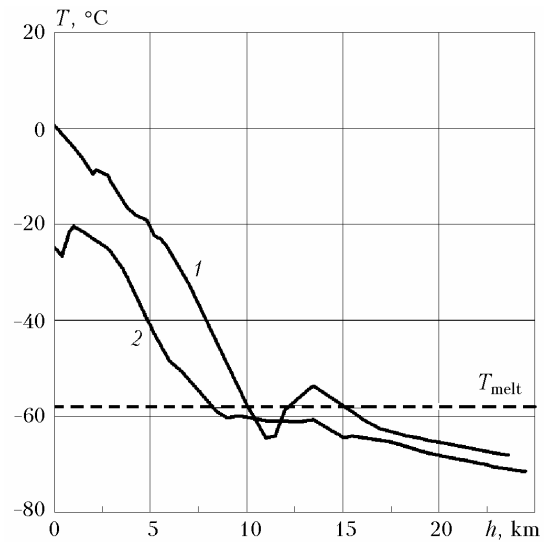


Fig. 5. Altitude dependence of atmosphere temperature on October 26 (1); 00:00 GTS on December 26, 2007 (2).

The level of atmosphere temperature in its turn determines heptil droplets evaporation rate. Figure 6 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.

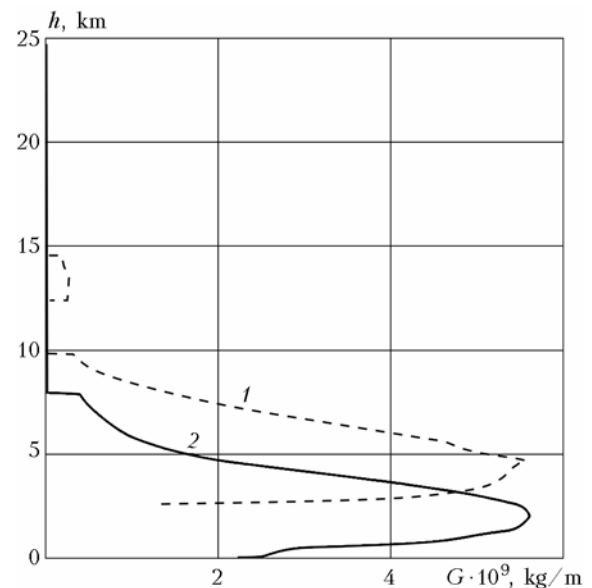


Fig. 6. UDMH droplets evaporation rate at different altitudes: October 26 (1); 00:00 GST on December 26, 2007 (2).

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°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.

Conclusion

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 formations.

Acknowledgements

This work was financially supported by Russian Foundation for Basic Research (Project No. 08-01-99025-r_ofi).

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