Modeling of the ground surface pollution with propellants

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The fall of the UDMH (unsymmetrical dimethylhydrazine) drops that are formed upon flowing-out of residual propellant from a rocket stage is considered. It is supposed that the propellant can flow out either discretely (at a single point) or continuously along the stage descent trajectory. The initial process of drop formation and the interactions among the falling UDMH drops are not considered. The drop fall trajectories and the final distribution of the UDMH mass precipitated on the earth's surface are calculated using real meteorological data.

Introduction

Among a wide variety of ecologically oriented problems of the Altai–Sayan region, an important problem is the pollution of the area of fall of the parts of space boosters launched from the Baikonur Cosmodrome with some residual propellant. As used booster stages are separated, their tanks still contain some propellant in the amount achieving several hundreds of liters. As the second stage enters the dense atmosphere at the altitude of 30–40 km, the tanks can become depressurized and the propellant is emitted into the atmosphere.

For more than 40 years, this situation affects adversely the people living in the booster impact areas. In this connection, the study of medical and biological consequences of the impact of residual propellant on the population in some areas of the Altai–Sayan region is of great practical interest.

The State Scientific Center of Virology and Biotechnology "Vector," Scientific Research Institute of Biochemistry SB RAMS, and the Institute of Computer Technologies SB RAS within the framework of the International Science & Technology Center study the clinical and epidemiological consequences of the long-term impact of these adverse factors on the human health. One of the tasks of this project is the development of mathematical models of pollution of the surface atmosphere and the ground surface with propellant and its combustion products upon falling of the used booster parts.

Unsymmetrical dimethylhydrazine (UDMH) $N_2H_2(CH_3)_2$ is a fuel, while nitrogen tetraoxide (NT) N_2O_4 serves an oxidizing agent. This propellant provides for the specific impulse almost 10% exceeding that of the mixture of the nitric acid and kerosene and only a little bit lower than that of the propellant based on NT and hydrazine.[1]

The UDMH propellant is still widely used in Russian cosmonautics. The UDMH is a toxicant of the first class of danger, having simultaneously the carcinogenic and mutagenic properties, and can be classified as a supertoxicant. For the atmospheric air, the recommended one-time maximum permissible concentration is 0.001 mg/m^3. UDMH is water-soluble and easily evaporable, which can lead to pollution of air, soil, surface and underground waters.

Propellant can be emitted along the entire descent trajectory.[2] A significant part of the propellant emitted at high altitudes must evaporate at the initial stage of aerobraking. The fraction of the evaporated part depends on the stage speed at the time of propellant emission, which decreases from 2–3 km/s at the altitude of 30 km to 0.1 km/s at the ground impact.[2]

The objective of this work was to construct a model of falling of UDMH drops produced from the residual propellant upon destruction of the used tanks of falling booster stages. This model should also account for the features of the boundary layer in modeling the drop sedimentation to the surface.

The simulation of the formation of the drop ensemble is a complicated problem, which cannot be solved completely nowadays. For this reason, we did not consider this process (as well as the authors of other papers[3–5]), and our calculations concern only the part of propellant, which remains once the formation of drops is completed. As in Refs. 3 and 4, we considered the exponential initial size distribution of drops with the distribution function $f(r) = A \exp(-1.56r)$, where r is the drop radius (mm).

It is assumed that the propellant is spread in air in the process of falling due to the atmospheric turbulent diffusion and the gravitational separation of different-size drops. The interaction between UDMH drops in air was neglected.

Modeling of drop fall and evaporation

It is assumed that in the reference coordinate system, in which the mean local wind velocity is

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zero, a drop falls vertically with an established (quasiequilibrium) speed. In simulation of the drop fall, the established drop speed v is determined iteratively at every time step with the use of the Stokes law[3,4,6]:

$$v = \frac{2\rho g r}{9\mu F/F_s},$$

where ρ is the UDMH density; g is the free-fall acceleration; μ is the dynamic viscosity of air; F/F_s is a correction factor:

$$F/F_s = \frac{\left[1+\varphi(\mathrm{Re})\right]\left(1+0.269\,\mathrm{We}^{1.7}\right)}{\left(1-M^2\right)^{0.5}};$$

$\mathrm{Re} = 2rv\rho/\mu$ is the Reynolds number; $\mathrm{We} = r\rho v^2/2\sigma$ is the Weber number; σ is the surface tension coefficient; $M = v/c$ is the Mach number; c is the speed of sound. The function $\varphi(\mathrm{Re})$ can be found elsewhere.[3,6]

The UDMH mass in a falling drop decreases gradually due to evaporation. This process is considered within the model described in Refs. 3–5. The rate of evaporation is determined by the diffusion removal of UDMH molecules from the drop into the atmosphere:

$$\frac{\mathrm{d}m}{\mathrm{d}t} = -4\pi D r\left(\rho_n^s - \rho_n^\infty\right)F_M,$$

where m is the drop mass; ρ_n^∞ and ρ_n^s are the UDMH vapor densities in the ambient air and near the drop surface. The diffusion coefficient of UDMH molecules in air D is calculated by the empirical equation accounting for the polarization of molecules.[5] The correction factor is

$$F_M = 1 + 0.28\,\mathrm{Sc}^{1/3}\,\mathrm{Re}^{1/2},$$

where $\mathrm{Sc} = \mu/\rho D$ is the Schmidt number.

Unlike the papers cited above, we also considered the possible effect of atmospheric moisture on the process of drop evaporation. UDMH is hygroscopic and mixes well with water in any proportion.[8] The presence of water retards UDMH evaporation. The parameters of aqueous UDMH solution at the arbitrary relative concentrations $0 < \xi < 1$ are unavailable in the literature. Therefore, we interpolated the parameters from the known limit values at $\xi = 0$ (pure UDMH) and $\xi = 1$ (pure water). The parameters for UDMH were borrowed from Refs. 3–5, 7, and 8, while those for water were taken from Refs. 9–11. Some equations for calculation of air properties were taken from the Russian State Standard No. 4401-81.[12]

For interpolation, we used the following limiting values (subscripts 1 and 2 correspond to UDMH and water, respectively):

surface tension coefficients (N/m):

$$\sigma_1 = 0.0588 - 0.0001157T_s,$$

$$\sigma_2 = 0.0756 - 0.000143(T_s - 273.15),$$

where T_s is the drop surface temperature (K);

density of pure UDMH (kg/m^3)

$$\rho_1 = 810 + 1.049(273.15 - T_s);$$

density of saturated UDMH vapor (kg/ m^3)

$$\rho_{sat1} = 0.007226\,\frac{\exp\left[(21.33T_s - 3950)/(T_s - 57.49)\right]}{T_s}.$$

The density of saturated water vapor was calculated by the equation from Ref. 9. The specific heats of evaporation (J/kg) are:

$$\lambda_1 = 583700\left[(522 - T_s)/224\right]^{0.36},$$

$$\lambda_2 = 2500000 - 2720(T_s - 273.15).$$

To estimate the heat of evaporation of molecules from the solution, we used the information about the typical energies of hydrogen bonds O–H–N and N–H–N. Since these energies vary widely in different compounds, this estimation is quite rough. To assess the possible influence of humidity, the heat of evaporation of UDMH molecules from the aqueous solution we used the following equation:

$$\tilde{\lambda}_1 = \lambda_1(1.4 - 0.4y_1),$$

where y_1 is the volume fraction of UDMH in the solution. The heat of evaporation of water molecules from the solution in these calculations was assumed independent of y_1.

The dependence of the saturated vapor pressure on the heat of evaporation was taken into account through the exponential Boltzmann factor. The most significant qualitative effect can be attributed to the increase in the heat of evaporation of UDMH molecules with the increase of the concentration of water molecules in the solution, which is connected with the transition from N–H–N hydrogen bonds to O–H–N hydrogen bonds.

Results and conclusions

Falling drops are subject to the horizontal wind drift, achieving 30–50 km for large drops falling from the 30-km altitude. In addition, the drop cloud can diffuse due to atmospheric turbulence. For a passive admixture, the diffusion shift can be about 2 km for 30 min.

The calculations showed that at a point-like emission the position of the maximum of UDMH deposited onto the surface in the drop form is determined by the fall of large drops with the initial radius of 2.0–3.0 mm. If the propellant flows out continuously (quasilinear source), these maxima form a line on the surface. At the uniform continuous UDMH flowing-out, the global maximum of the UDMH concentration is observed at the place of stage impact, because in this case UDMH does not evaporate and diffuse due to the turbulent diffusion.

To illustrate the efficiency of the model, we have carried out test calculations with the use of telemetry

data for the stage fall trajectory and meteorological data for Novosibirsk at 00 GMT on April 28, 1999.

Thirty points of propellant emission along the stage fall line were considered. Emissions occurred with the interval of 5 s. The last emission took place 5 s before the stage impact. For each emission, the fall of 14 drops with the initial radii from 3.0 to 0.4 mm (with the step of 0.2 mm) was simulated.

The calculated fall lines of the drops initially consisting of pure UDMH are shown in Figs. 1 and 2. Figure 2 also depicts the Gaussian distributions of the UDMH mass deposited onto the surface with these drops as calculated with the allowance for the drop evaporation and the spread of the drop ensemble due to the atmospheric turbulent diffusion (in the approximation of passive drops).

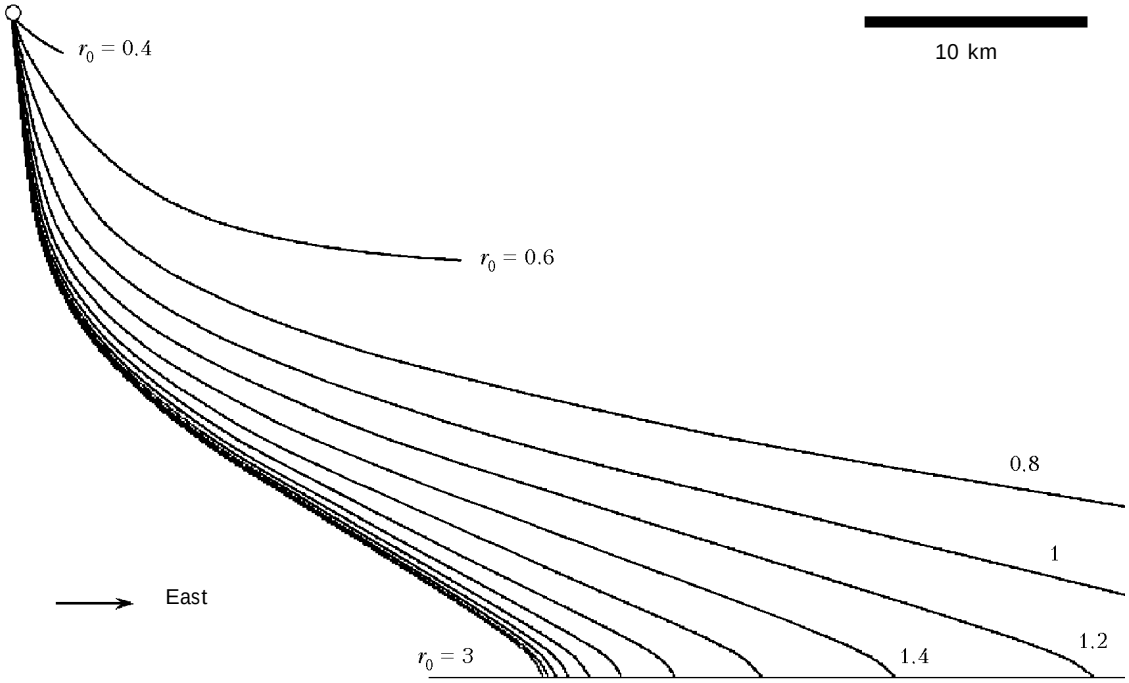

Fig. 1. Fall lines of drops falling from the 30-km altitude onto the surface; r_0 is the initial drop radius, mm.

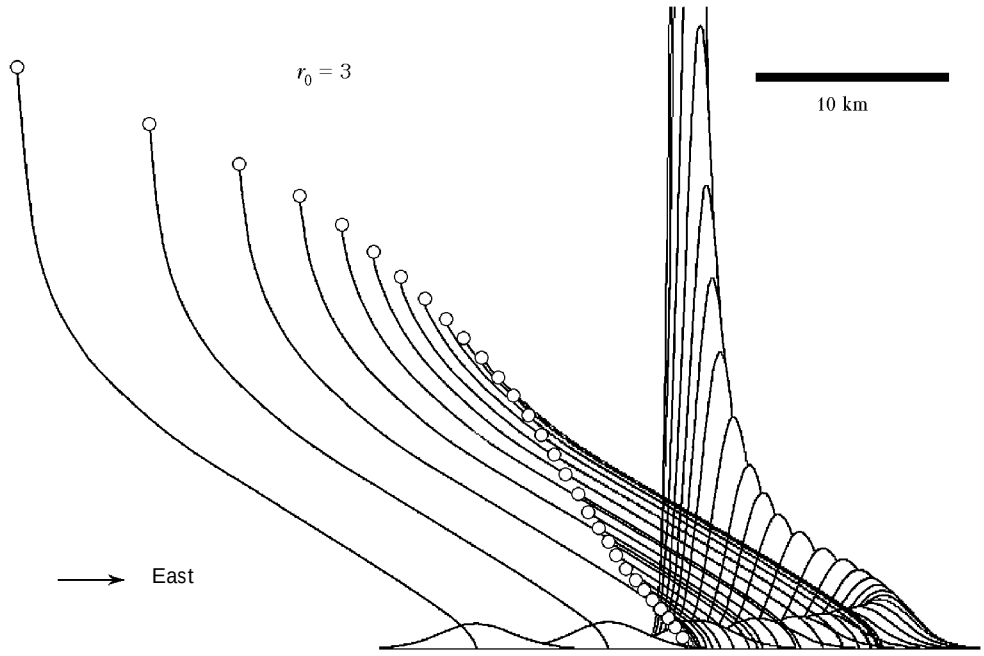

Fig. 2. Fall lines of drops with the initial radius of 3 mm emitted from a tank with the interval of 5 s. The corresponding Gaussian distributions of the UMDH mass deposited onto the surface are shown for each drop.

UDMH drops with the initial radius of 3 mm falling from the 30-km altitude reach the ground in 28.2 min, shifting by 23.7 km to the east and by 19.0 km to the south. During the fall, the drop radius decreases to 1.56 mm, and the relative mass fraction of water in the drop amounts to 0.2. Thus, only 11% of the initial UDMH mass reaches the ground in this drop.

Drops falling from the following parts of the stage fall trajectory reach the ground, having greater size and smaller relative fraction of water in their composition. Drops with the smaller initial radius have the lower fall rate and the longer evaporation, and therefore they are shifted to the longer distances.

Figures 3 and 4 depict the distributions of the surface density of UDMH deposited onto the surface in the form of drops. The results shown in Fig. 3 were obtained with the neglect of atmospheric humidity.

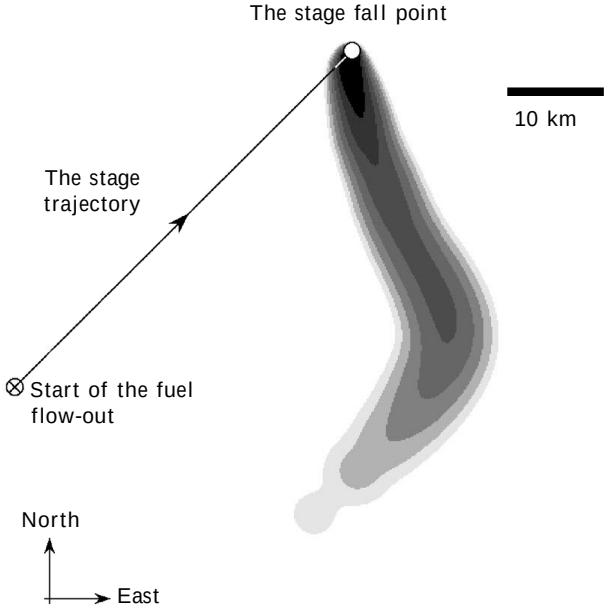

Fig. 3. Density distribution of UDMH deposited onto the surface as estimated neglecting the humidity. Grey-color grades correspond to the fourfold density variations. In the case of uniform flowing-out, 5.2% propellant reaches the ground.

The results calculated with the allowance for humidity are shown in Fig. 4. Each grey-color grade in Figs. 3 and 4 corresponds to the fourfold decrease of the density. The white color of the background corresponds to the UDMH concentration, which is 4^7 or 16 384 times lower than the maximum concentration shown by the black color.

At the total mass of emitted propellant (or the mass rest after the initial aerobraking) of 300 kg, the maximum density is $6.2 \cdot 10^{-6}$ kg/m^2 (see Fig. 3) and $6.4 \cdot 10^{-6}$ kg/m^2 (see Fig. 4) in the area colored in black.

The model described above will be used to assess the zone polluted by the residual propellant in the areas of impact of the used stages of space boosters launched from the Baikonur Cosmodrome.

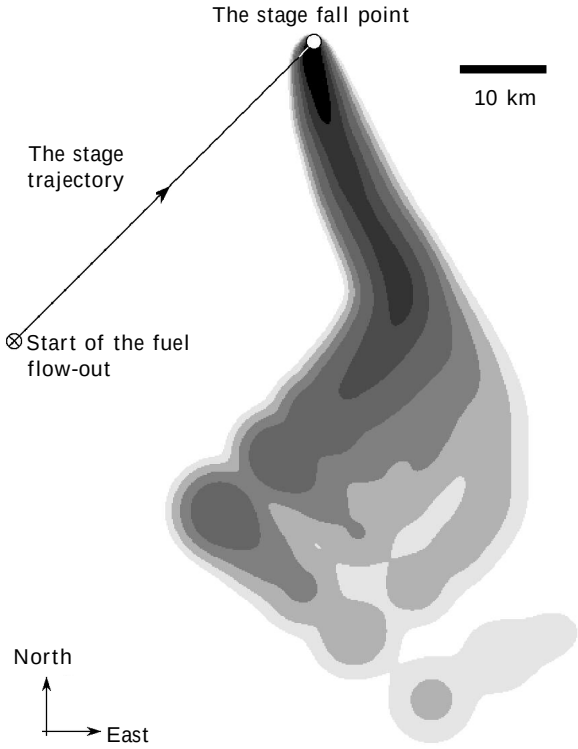

Fig. 4. Density distribution of UDMH deposited onto the surface with allowance for humidity. Grey-color grades correspond to the fourfold density variations. In the case of uniform flowing-out, 8.7% propellant reaches the ground.

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