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Numerical simulation of clouds formation based on the power of explosion estimated by the sizes of the funnel

Abstract. This paper considers numerical modeling of cloud formation under the action of buoyancy force, taking into account the turbulent mixing and the adiabatic expansion. Based on the solution of the three-dimensional filtered non-stationary Navier-Stokes equation, the continuity equation, the concentration equation, the enthalpy equation, and the equation of state for compressible media numerical modeling of cloud formation is carried out. The modified solver is based on the library Open Foam of solution of mathematical physics problems. To close the basic equations the viscosity model of turbulence is used. Numerical modeling of the formation of clouds formed at ground explosion of the launch vehicle "Proton-M" 2nd July 2013, shows the dependence of the fireball height from the thermodynamic parameters in the atmosphere. Comparison of the cloud rise height as a function of the explosion power with the analytic formula of Satton confirmed the applicability of the mathematical model used to the cloud formation problem in a surface explosion of a launch vehicle. The explosion power is calculated from the funnel size.

Key words: explosion, Proton-M, cloud formation, turbulence, Navier-Stokes equation, finite-volume method, large eddy simulation, fireball.

In this paper the numerical modeling of cloud formation under the action of buoyancy force is considered. The air temperature at the initial moment of the vortex ring of the cloud is very large, and over time, it falls due to adiabatic expansion, since the pressure decreases with altitude and due to turbulent mixing of heated and cold air. Under the force of buoyancy fireball heated air will rise in the atmosphere until the temperature, density due to convective and diffusive mixing of external and internal gas components of the heated and cold air is equal.

The temperature cooling due to thermal radiation can be neglected, since the length of the path of radiation is much larger than the dimensions of cloud.

Numerical modeling of the cloud formation is based on the solution of the three-dimensional filtered non-stationary Navier-Stokes equation, the continuity equation, the concentration equation, the enthalpy equation, and the equation of state for compressible media. To close the basic equations a viscous model of turbulence is used. The main problem in this task is correct the description of the turbulent transport processes. In this paper, an attempt to solve this problem by using large eddy simulation is made.

Formulation of the problem

There is a fiery half sphere at the initial moment of time at the earth surface, denoted by field G , radius R , initial temperature of ball T_1 , and initial three-dimensional density of dry air's gas phases ρ_d , and humid air ρ_w , ambient temperature T_0 (picture 1).

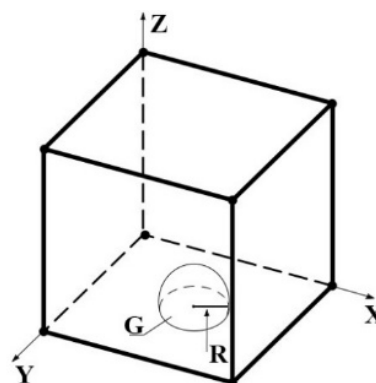


Figure 1 – Schematic illustration of the problem statement

To solve the problem the following filtered equations are used:

The equation of continuity:

$$\frac{\partial \bar{\rho}_m}{\partial t} + \nabla \cdot (\bar{\rho}_m \bar{u}_m) = 0, \tag{1}$$

where u_m is velocity of the gas phase mixture, $\rho_m = \rho_w + \rho_d$ is air density, $\nu_m = \frac{\mu_m}{\rho_m}$ is dynamic viscosity, $\mu_m = \mu_* \left(\frac{T}{T_*} \right)^w$, where μ_* is the value of dynamic viscosity at temperature T_* , $\rho_d = \sum_{\alpha=1}^{N_\alpha} S_\alpha \rho_\alpha$; $\sum_{\alpha=1}^{N_\alpha} S_\alpha = 1$ is three-dimensional density of dry air's gas phase, $\rho_w = \sum_{\beta=1}^{N_\beta} S_\beta \rho_\beta$; $\sum_{\beta=1}^{N_\beta} S_\beta = 1$ three-dimensional density of the water vapors gas phase, $\rho_\alpha = \rho_{*\alpha} (1 - \gamma(T - T_*))$, $\alpha = 1, \dots, N_\alpha$; $\rho_\beta = \rho_{*\beta} (1 - \gamma(T - T_*))$, $\beta = 1, \dots, N_\beta$, also $\rho_{*\alpha}, \rho_{*\beta}$ are density of dry air's gas components and moist air, respectively, at $T_* = 20^\circ C$.

The concentration equation:

$$\begin{aligned} \frac{\partial (\rho_m S_\alpha)}{\partial t} + \nabla \cdot (\rho_m u_m S_\alpha) &= -\nabla \cdot G_\alpha, \\ \frac{\partial (\rho_m S_\beta)}{\partial t} + \nabla \cdot (\rho_m u_m S_\beta) &= -\nabla \cdot G_\beta, \end{aligned} \tag{2}$$

where $G_\alpha = \bar{\rho}_m (\overline{S_\alpha u_m} - \bar{S}_\alpha \bar{u}_m) = -\frac{\mu_t}{Pr_t} \nabla \bar{S}_\alpha$, $\alpha = 1, \dots, N_\alpha$, $G_\beta = \bar{\rho}_m (\overline{S_\beta u_m} - \bar{S}_\beta \bar{u}_m) = -\frac{\mu_t}{Pr_t} \nabla \bar{S}_\beta$, $\beta = 1, \dots, N_\beta$ describe the contribution of the sub-grid turbulent scales for gas components concentration equation.

The motion equation:

$$\begin{aligned} \frac{\partial (\rho_m u_m)}{\partial t} + \nabla \cdot (\rho_m u_m \otimes u_m + \rho_m \mathbf{T}_r) &= \\ = -\nabla p + \nabla \cdot \mathbf{T} + \rho_m \mathbf{g} - \nabla \cdot \mathbf{B} \end{aligned} \tag{3}$$

where $\mathbf{B} = \bar{\rho}_m (\overline{u_m \otimes u_m} - \bar{u}_m \otimes \bar{u}_m) = \frac{2}{d} K_t \mathbf{I} - 2\mu_t \mathbf{S}_m$ - subgrid tensor responsible for small-scale structures,

that need to be modeled, \mathbf{g} - acceleration occurs under the gravity action, \mathbf{T} - stress tensor of gas phase, t - time, p - pressure.

The enthalpy equation:

$$\begin{aligned} \frac{\partial (\rho_m h_m)}{\partial t} + \nabla \cdot (\rho_m h_m u_m) + \nabla \cdot (q - \mathbf{T} \cdot u_g) &= \\ = \frac{\partial p}{\partial t} - \frac{\partial (\rho_m K_m)}{\partial t} - \nabla \cdot (\rho_m K_m u_m) + & \tag{4} \\ + \rho_m (\mathbf{g} \cdot u_m) - \nabla \cdot (Q + Q_K) \end{aligned}$$

where $Q = \bar{\rho}_m (\overline{h_m u_m} - \bar{h}_m \bar{u}_m) = -\frac{\mu_t}{Pr_t} \nabla \bar{h}_m$, $Q_K = \bar{\rho}_m (\overline{K_m u_m} - \bar{K}_m \bar{u}_m) = -\frac{\mu_t}{Pr_t} \nabla \bar{K}_m$ - describe the contribution of the sub-grid turbulent scales [1, 2], Pr_t - turbulent Prandtl number, μ_t - turbulent viscosity, h_m - enthalpy of gas mixture, heat flux in the gas phase - $q = -k_g \Delta T$, where $k_g = \sum_{i=1}^I \chi_i k_i$, k_i - i -th component's conductivity, T - temperature, $K_m = \frac{1}{2} [u_m]^2$ - kinetic energy per unit mass of the gas phase.

The temperature equation:

$$T = \frac{h_m}{\frac{1}{\rho_m} \sum_{i=1}^I \rho_i C_i + \frac{1}{\rho_m} \sum_{i=1}^I \rho_i R_i} \tag{5}$$

where C_i - heat capacity of the gas phase at constant volume.

The equation of ideal gas' state is:

$$\begin{aligned} P &= \frac{R_*}{M_{rd}} \rho_d T + \frac{R_*}{M_{rw}} \rho_w T = \\ &= R_* T \left(\frac{\rho_d}{M_{rd}} + \frac{\rho_w}{M_{rw}} \right). \end{aligned} \tag{6}$$

where $R_* = 8.3144598$, $M_{rd} = \sum_{\alpha}^{N_\alpha} S_\alpha M_{r\alpha}$,

$M_{rw} = \sum_{\beta}^{N_\beta} S_\beta M_{r\beta}$.

Initial conditions:

$$u_i(x_1, x_2, x_3, t = 0) = u_0(x_1, x_2, x_3), (x_1, x_2, x_3) \in G,$$

$$u_i(x_1, x_2, x_3, t = 0) = 0, (x_1, x_2, x_3) \notin G,$$

$$T(x_1, x_2, x_3, t = 0) = T_1, (x_1, x_2, x_3) \in G,$$

$$T(x_1, x_2, x_3, t = 0) = T_0, (x_1, x_2, x_3) \notin G,$$

$$S_\alpha(x_1, x_2, x_3, t = 0) = \frac{\rho_\alpha}{\rho_m}, \alpha = 1, \dots, N_\alpha$$

$$S_\beta(x_1, x_2, x_3, t = 0) = \frac{\rho_\beta}{\rho_m}, \beta = 1, \dots, N_\beta,$$

Boundary conditions:

$$\frac{\partial u_i}{\partial n} = 0, \frac{\partial S_\alpha}{\partial n} = 0, \frac{\partial S_\beta}{\partial n} = 0, \frac{\partial T}{\partial n} = 0, i = 1, 2, 3, \\ \alpha = 1, \dots, N_\alpha, \beta = 1, \dots, N_\beta.$$

The algorithm for determining the initial value of fireball's temperature

The equation of total energy consists specific internal energy and kinetic energy. Suppose that in this problem the kinetic energy is zero.

$$E = U \quad (7)$$

where $E = 0,25 \cdot q \cdot t_{ex}$ - explosion energy; t_{ex} - explosion time; q - explosion power.

One-third of the energy released during the explosion is emitted in radiation form [3]. As a result, the energy enclosed in the fireball at the rise beginning is approximately one quarter of total explosion energy.

Specific internal energy in the adiabatic process is expressed by:

$$U = C_V(T_1 - T_0) \quad (8)$$

where C_V - is heat capacity of gas with a constant volume, T_1 is ambient temperature for different values of fireball's initial temperature T_0 .

Substituting equation (8) into equation (7), the initial value of the fireball's temperature is obtained:

$$T_0 = \frac{E}{C_V} + T_1.$$

Numerical method

Three dimensional numerical simulation of equation (1) - (6) is performed with indicated initial and boundary conditions to obtain non-stationary fields of unknown variables.

The numerical algorithm based on the finite volume method on unstructured grid using the OpenFOAM class library for C++ with an open GPL license is implemented. Using C++ templates, the OpenFOAM library allows to quickly creating effective solvers and utilities for pre and post processing of modeling results due to the high level of abstraction. Classes and functions in the OpenFOAM library have implicit means for parallelizing computational procedures, due to the numerical calculation on multiprocessor computing systems does not require specific adaptations in the program code. In the finite volume method [4], partial differential equations are integrated over the volume of arbitrary cell, after the Gauss-Ostrogradsky theorem is used to translate volume integrals into surface integrals. It is necessary to interpolate unknown values on each face of finite volume, when calculating flows across finite volume boundaries. Such characteristics as accuracy and stability depend on the interpolation method's choice. Integration over time using the Crank-Nicholson scheme is carried out, the Courant number was maintained at 0.5.

Both for convective and diffusion terms implicit schemes to ensure the stability of numerical calculations were used. To bind the velocity and pressure fields the PISO procedure was used, as well as to implement the law of conservation of mass [5]. In the equations of motion and mass conservation, the explicit representations of pressure and gravity fields are used. Spatial discretization has second-order accuracy. The PISO algorithm consists of one-step of predictor and several steps of correctors. Using the pressure field from the previous time layer in the predictor step an intermediate velocity field is found. Velocity and pressure fields are corrected to increase the accuracy and reduce the mass defect in the conservation equation at each step of the corrector. The system of linear algebraic equations obtained as a result of the transport equation discretization is solved by the conjugate gradient method with the precedent of Khaletsky for the pressure equation and by the method of bi-conjugate gradients with a preconditioner of incomplete LU factorization.

Simulation results

There are results of numerical simulation of cloud formation and dynamics, formed during a surface explosion of a launch vehicle. Numerical simulation of the gas-dust cloud formation stage in the first minutes of the accident in a cubic area with the physical size of the cube edge 1280 m and the calculated grid 128x128x128 was carried out. Ground explosion is accompanied by the funnel formation at Figure 2. Funnels dimensions depend mainly on the explosion power and soil-soil type.

The explosion power and depth of the funnel are related by the [6, 7]:

$$q = K_B W^3 (0,4 + 0,6n^3) \quad (9)$$

where q – explosion power; $K_B = 1,35$ - design specific consumption of explosives, kg / m³; $W=5$ – depth of the funnel, m; $n=2$ – explosion index.

Formula (9) allows to calculate the explosion power at a known depth of the funnel, it turned out $q=0,878$ t.



a)



b)

Figure 2 – a) Explosion at the emergency fall place (30 seconds);
b) formation of the cloud (1 minute after the explosion)

At the first seconds of the accident cloud takes on a mushroom shape, where a vortex ring on the upper part is observed, as can be seen from figure 3. At the initial time, the vortex ring's temperature is large and equal to 1800 K, for 5.5 seconds the temperature drops substantially to 400 K due to adiabatic expansion and turbulent mixing of the cloud's heated air and the environment's cold air. The drop in the cloud's temperature after 5.5 seconds occurs at a lower rate, because at these times the temperature changes due to turbulent mixing.

The fireball of heated air rises to the atmosphere until the temperature, the density due to convective and diffusive mixing of external and internal gas components of the heated and cold air are equal, under the influence of buoyancy force. Effect of thermal radiation is not taken into account while performing numerical simulation. Figure 3 shows the distribution dynamics of the mixture concentration concentration in the cloud. Figure 4 shows the change graphs in the height of the cloud rise, maximum temperature in the cloud, volume of the cloud as a time function.

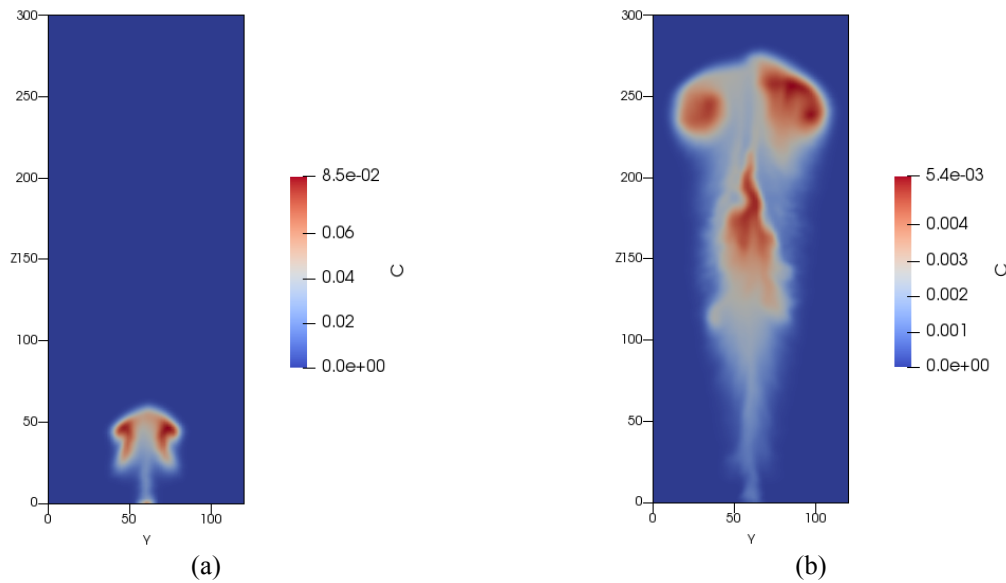


Figure 3 – Distribution dynamics of the mixture concentration field at the initial value of explosion energy $E = 3.67 \cdot 10^9$ J in cross section $x = 60$ m: a) $t = 5$ sec; б) $t = 35$ sec.

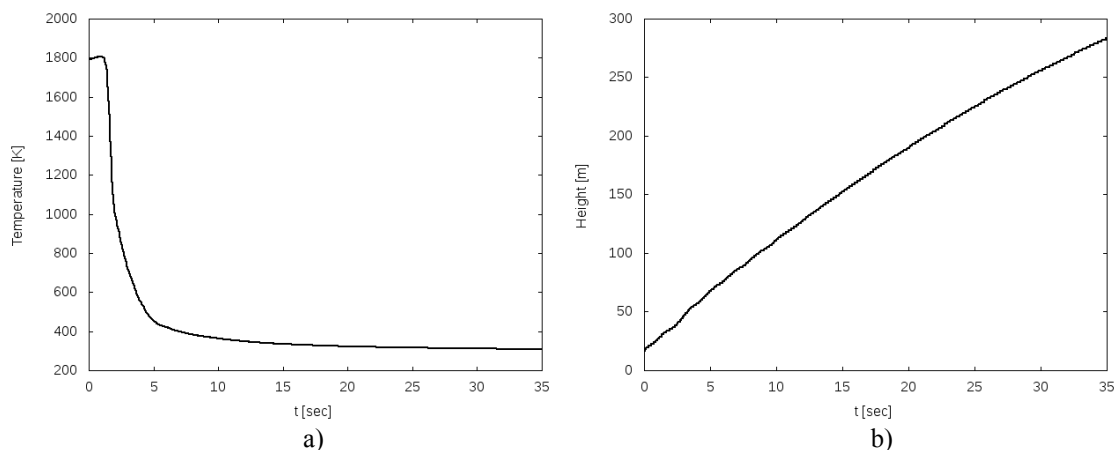


Figure 4 – Change of a) temperature; б) the formed cloud height with the explosion power $q=0.878 \tau$.

Conclusion

The results of numerical simulation of cloud formation are obtained. The following geometric characteristics of the cloud raised as a result of the ascent are determined: the height of the uplift of the cloud, the volume of the cloud, the shape of the vortex ring in the cloud. Comparison of the cloud rise height as a function of the explosion power with the analytic formula of Sattouf confirmed the applicability of the mathematical model used to the cloud formation problem in a surface explosion of a

launch vehicle. The explosion power is calculated from the funnel size.

In conclusion, we note that the results of this study allow us to estimate the geometric characteristics of raised cloud, the concentration of gas components mixture in the cloud at different instants of time. Such an opportunity is invaluable in absence of experimental data on the cloud formed as a result of an accident. The obtained results allow conducting a primary assessment of the accident impact on the environment.

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