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# Large eddy simulation the evolution of the cloud explosion of a launch vehicle

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**Abstract** In this paper, the evolution of an explosion cloud under the influence of buoyancy force is considered, taking into account turbulent mixing and adiabatic expansion. Numerical simulation on the basis of the solution of the three-dimensional filtered non-stationary Navier-Stokes equation, the continuity equation, the concentration equation, the enthalpy equation, the equation of state for compressible media is carried out. The modified solver is based on the OpenFOAM mathematical physics library. To close the basic equations a viscous model of turbulence is used. The dependence of the cloud lifting height of the launch vehicle explosion on the thermodynamic parameters is obtained based on the large eddy simulation.

## Introduction

Emergency fall launch vehicles are often accompanied by ground blast, which yields a gas-dust cloud. The impossibility of carrying out experimental measurements of the mechanical and chemical composition of the cloud, its temperature, interaction with the environment, in connection with the transience of the process of formation and propagation of the cloud, necessitate the use of methods of mathematical modeling. The study of the process of raising an explosion cloud under the influence of Archimedes' force, taking into account turbulent mixing and adiabatic expansion, despite the large number of publications on this topic, remains an urgent task for researchers.

For the first time, the problem of lifting the cloud of an atomic explosion was considered in [1], [2] by Satton and Machta, where it is assumed that the rise of the cloud is caused by Archimedes' force, and the cooling occurs as a result of adiabatic expansion and mixing with the surrounding air. Circulation in the cloud and the influence of inertia are not taken into account, as well as an analytical method for determining the values of the maximum lift height of the cloud by launch vehicle explosion .

In [3], [4], the process of propagation of a turbulent gas jet in a medium of a different density and the initial section of a turbulent jet of a compressible gas were investigated,where on the surface of the explosion cloud turbulent mixing of heated air inside the ring occurs and of cold ambient air.

The problem of the motion of a vortex ring formed after an explosion under the action of gravity was theoretically investigated in [5], where the case of a small density difference inside and outside the cloud was considered, as well as the case when the density difference is large.The volume of hot air formed after an explosion from a shock wave, clouds of the launch vehicle explosion, after increasing to a certain size, tends upward, forming a vortex ring. In the case when the cloud is formed at the surface of the Earth, its rise is accompanied by the raising of a dust column giving a mushroom shape. The main acting force for raising the cloud is Archimedes' power, which arises at different density of air, both inside the cloud and outside the cloud, in the atmosphere. But, in addition to the strength of Archimedes, because of the existence of a vortex ring of circulation, Zhukovsky's force acts on the cloud, directed perpendicularly to the direction of the velocity of movement of the element of the ring. The horizontal component of this force stretches the vortex ring to the sides, and the vertical component - somewhat inhibits the lifting of the ring. The air temperature at the beginning of the rise is large, then falls due to adiabatic expansion. As a result of the study, the dependence of the vertical and horizontal components of the velocity of motion on time, as well as the geometric dimensions of the cloud depending on the power of the explosion were obtained.

The study of the evolution of large-scale thermals in the inhomogeneous atmosphere, produced by powerful explosions, within the framework of the Boussinesq approximation made in the work in 1987 [6].

In the above mentioned works [5], [6] Boussinesq approximation was used, in which the density is considered constant in all terms of the equation of motion, where the density is proportional to the temperature gradient. However, Boussinesq approximation is applicable only for description of flows with relatively small temperature changes and small values of hydrostatic compressibility parameter [7].

With the advent of relatively affordable computing devices, works appeared in which more complex models [7], [8], [9] based on the Navier-Stokes equations for compressible gases were used to describe the process of lifting the explosive cloud. Physically, the use of compressible formulation in equations leads to more adequate results, since density is not always a linear function of the temperature gradient.

In this paper, we consider the raising of the launch vehicle explosion cloud under the influence of Archimedes ' force, taking into account turbulent mixing and adiabatic expansion. The air temperature at the initial moment of the vortex ring is very high, over time it falls due to adiabatic expansion, i.e. reducing the pressure with height and due to turbulent mixing of heated and cold air. Under the influence of Archimedes force, clouds of explosion of heated air will rise into the atmosphere until the temperature is equalized, the density of the gas components of the external and internal heated and cold air due to convective and diffusive mixing. The cooling temperature due to thermal radiation can be neglected, because the length of the radiation path is much larger than the cloud.

Numerical modeling of cloud formation is based on the solution of three-dimensional filtered unsteady Navier-Stokes equation, continuity equation, concentration equation, enthalpy equation of state for compressible media.The viscosity turbulence model is used to close the main equations. The main problem in this paper is the correct description of turbulent transport processes. The explosion power is calculated from the size of the funnel.

The results of numerical modeling of the cloud formation formed during the ground explosion of the Proton-M launch vehicle on July 2, 2013 in the position area of the Baikonur cosmodrome are presented. The dependence of the cloud lifting height in the atmosphere on thermodynamic parameters is shown. The obtained results of the simulation that determines the height of rise of the cloud corresponds to the results of the work of [5],under a low power of the explosion.

### Problem statement

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 $T_0$, and initial three-dimensional density of dry air's gas phases $\rho_d$, and humid air $rho_w$, ambient temperature $T_1$ (Fig. 2).

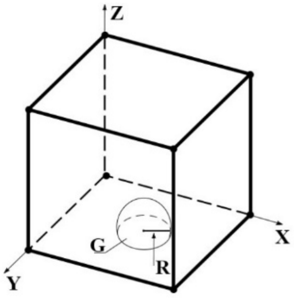


**Figure 1.** Schematic illustration of the problem statement.

The following filtered equations are used to solve the problem under consideration: The equation of continuity:

$$\frac{\partial \rho_m}{\partial t} + v(\rho_m u_m) = 0 \tag{1}$$

where $u_m$ is velocity of the gas phase mixture, $\rho_m = \rho_w + \rho_d, u_m = \frac{\nu_m}{\rho_m}$ is air density, $v_m = \frac{\nu_m}{\rho_m}$ is dynamic viscosity, $\nu_m = \nu_* \left(\frac{T}{T_*}\right)^w$, where $\nu_*$ 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 airs gas phase, $\rho_w = \sum_{\beta=1}^{N_\beta} S_\beta \rho_\beta$; $\sum_{\beta=1}^{N_\beta} = 1$ three-dimensional density of the water vapors gas phase, $\rho_\alpha = \rho_{*\alpha}(1-\gamma(T-T_*))$,

$\alpha = 1, \ldots, N_\alpha$; $\rho_\beta = \rho_{*\beta}(1 - \gamma(T - T_*))$, $\beta = 1, \ldots, N_\beta$, also $\rho_{*\alpha}, \rho_{*\beta}$ are density of dry air's gas components and moist air, respectively, at $T_* = 20^0 C$.

The concentration equation:

$$\begin{aligned} \frac{\partial(\rho_m S_\alpha)}{\partial t} = \nabla(\rho, u_m S_\alpha) = 0, \alpha = 1, \ldots, N_\alpha \\ \frac{\partial(\rho_m S_\beta)}{\partial t} = \nabla(\rho, u_m S_\beta) = 0, \beta = 1, \ldots, N_\beta \end{aligned} \tag{2}$$

The equation of motion:

$$\frac{\partial(\rho_m u_m)}{\partial t} + \nabla(\rho_m u_m \otimes u_m + \rho_m T_r) = -\nabla p + \nabla T + \rho_m g \tag{3}$$

where $g$- acceleration occurs under the gravity action, $T$-– stress tensor of gas phase, $t$ -– time, $p$ -– pressure.

The enthalpy equation:

$$\begin{aligned} \frac{\partial(\rho_m h_m)}{\partial t} + \nabla(\rho_m h_m u_m) + \nabla(q - T \cdot u_g) = \\ = \frac{\partial \rho}{\partial t} - \frac{\partial(\rho_m K_M)}{\partial t} - \nabla(\rho_m K_m u_m) + \rho_m(g u_m) \end{aligned} \tag{4}$$

where $h_m$ - enthalpy of gas mixture, heat flux in the gas phase – $-q = -k_g \Delta T$, here $k_i$ - $i$ -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 $C_i$ - specific heat of gas phase at constant.

The pressure equation: The equation of ideal gas' state is:

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

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:

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

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

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

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

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

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

Boundary conditions:

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

## 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.

$$E = U \tag{7}$$

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:

$$U = C_v(T_1 - T_0) \tag{8}$$

where $C_v$ is heat capacity of gas in processes 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), there is obtained the initial value of the fireball's temperature:

$$T_0 = \frac{E}{C_v} + T_1 \tag{9}$$

## Large eddy simulation

Applying the filter to the basic equations (1) - (6), the following equations are obtained [10], [11]:

The equation of continuity:

$$\frac{\partial \overline{\rho}_m}{\partial t} + \nabla(\overline{\rho}_m \cdot \overline{u}_m) = 0 \tag{10}$$

The concentration equation:

$$\begin{aligned} &\frac{\partial(\rho_m S_\alpha)}{\partial t} + \nabla(\rho, u_m S_\alpha) = -\nabla G_\alpha, \alpha = 1, \ldots, N_\alpha \\ &\frac{\partial(\rho_m S_\beta)}{\partial t} + \nabla(\rho, u_m S_\beta) = -\nabla G_\beta, \beta = 1, \ldots, N_\beta, \end{aligned} \tag{11}$$

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

The equation of motion:

$$\frac{\partial(\rho_m u_m)}{\partial t} + \nabla(\rho_m u_m \otimes u_m + \rho_m T_r) = -\nabla p + \nabla \cdot T + \rho_m g - \nabla \cdot B \qquad (12)$$

where $B = \overline{\rho_m} = (\overline{u_m \otimes u_m} - \overline{u_m} \otimes \overline{u_m} = \frac{2}{d}K_t I - 2\mu_t S_m$ - subgrid tensor responsible for small-scale structures, that need to be modeled.

The enthalpy equation:

$$\begin{gathered}\frac{\partial(\rho_m h_m)}{\partial t} + \nabla(\rho_m h_m u_m) + \nabla(q - T \cdot u_g) = \\ = \frac{\partial\rho}{\partial t} - \frac{\partial(\rho_m K_M)}{\partial t} - \nabla(\rho_m K_m u_m) + \rho_m(g u_m) - \nabla(Q + Q_k)\end{gathered} \qquad (13)$$

where $Q = \overline{\rho}_m(\overline{h_m u_m} - \overline{h}_m\overline{u}_m) = -\frac{\mu_t}{Pr_t}\Delta\overline{h}_m$, $Q_K = \overline{\rho}_m(\overline{K_m u_m} - \overline{K}_m\overline{u}_m) = = -\frac{\mu_t}{Pr_t}\Delta\overline{K}_m$, describe the contribution of subgrid turbulent scales [12], [13] , $Pr_t$- turbulent Prandtl number, $\mu_t$- turbulent viscosity.

## Numerical method

Three dimensional numerical simulation of equation (10) - (13) is performed with indicated initial and boundary conditions to obtain non-stationary fields of unknown variables. The implementation of the numerical algorithm is based on the finite volume method on unstructured grid using the OpenFOAM class library for C++ with an open GPL license. Using C++ templates, the OpenFOAM library allows to quickly create 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 [14], 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 is carried out using the Crank-Nicholson scheme, the Courant number was maintained at 0.5.

Both for convective and diffusion terms implicit schemes were used to ensure the stability of numerical calculations.

The PISO procedure was used to bind the velocity and pressure fields, as well as to implement the law of conservation of mass [15]. In the equations of motion and mass conservation are used explicit representations of pressure and gravity fields. Three-dimensional sampling has a second order of accuracy. The PISO algorithm consists of one step of predictor and several steps of proof-readers. An intermediate velocity field is found using the pressure field from the previous time layer in the predictor step. 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.

The algorithm of numerical solution is developed as follows:

1. Solving the conservation equation for mixture density by an explicit method using flows from the previous time layer.
2. Solution of the transport equation for gas components.
3. Solving the momentum conservation equation using the pressure field from the previous iteration.
4. Solving the enthalpy transfer equation using the pressure field from the previous iteration.
5. The solution of a Poisson equation for the pressure.
6. Modification of density and velocity fields based on the new pressure field.
7. Resume iteration from step 5 to reduce the mass defect in the mass conservation equation.
8. The calculation of the subgrid viscosity.
9. Assess the accuracy of the solution and move to step 2 if necessary.

## Simulation results

There are results of numerical simulation of cloud formation and dynamics, formed during a surface explosion of a carrier rocket. Numerical simulation of the gas-dust cloud formation stage in the first minutes of the accident was carried out in a cubic area with the physical size of the cube edge 1280 m and the calculated grid $128 \times 128 \times 128$. Ground explosion is accompanied by the funnel formation at Fig.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]:

$$q = K_B W^3 (0.4 + 0.6 n^3) \tag{14}$$

where $q$ – explosion power; $K_B = 1,35$ - design specific consumption of explosives, $kg/m^3$; $W = 5$ – depth of the funnel, $m$;$n = 2$– explosion index. Formula (14) allows to calculate the explosion power at a known depth of the funnel, it turned out q=0,878 t.

The maximum lifting height (km) of the explosion cloud is determined by The setton formula [1]-[5]: $H = 0.665 q^{0,276}$.

**Table 1.** Meteorological parameters for 02.07.2013 (08:00), platform 92 (altitude about 100 m)

| Height, m | Air Temperature, C | Air Humidity, % | Atmospheric pressure, mmHg | Wind Direction, Deg. | Wind Speed, m/s |
|---|---|---|---|---|---|
| 10 | 18.6 | 45 | 738.5 | 10 | 6-8 |
| 20 | | | | 20 | 7-8 |

**Table 2.** The parameters of the explosion of the launch vehicle

| | |
|---|---|
| stage number of launch vehicle | 1+2+3 |
| The remainder of the propellant at the time of the explosion (UDMH + at), t | 0.703 |
| An indicator of the impact of the explosion (n) | 2 |
| The power of the explosion, t | 0.878 |
| The depth of the crater, m | 5 |
| The radius of the crater, m | 10 |
| The diameter of the crater, m | 20 |
| The volume of the crater, m | 785.4 |
| Mass ejected from the funnel of the soil, t | 1178.2 |
| Shaft height (parapet) funnel, m | 1.3 |
| The radius of the cloud of explosion, m | 2.6 |
| The volume of the cloud of explosion, m | 74.05 |
| The energy of the explosion, $10^9$ J. | 3.67 |
| Raising the height of the clouds, m | 288 |

**Table 3.** Physico-chemical properties of cloud gases

| No. | Name | Molar mass, $g/mol$ | Density at $0^0C$, $kg/m^3$ | Kinematic viscosity, $m^2/s$ | Dynamic viscosity, PA at $0^0C$ | Diameter, m | Fraction, % |
|---|---|---|---|---|---|---|---|
| 1 | Carbon monoxide | 28.01 | 1.25 | $1329.6 \cdot 10^{-8}$ | $1662 \cdot 10^{-8}$ | $0.32 \cdot 10^{-9}$ | 15 |
| 2 | Carbon dioxide | 44.01 | 1.9768 | $693.039 \cdot 10^{-9}$ | $1370 \cdot 10^{-8}$ | $0.33 \cdot 10^{-9}$ | 1.95 |
| 3 | Nitrogen | 28.01456 | 1.251 | $2.053 \cdot 10^{-8}$ | $1660 \cdot 10^{-8}$ | $0.3 \cdot 10^{-9}$ | 78 |
| 4 | Nitric oxide | 30.00061 | 1.3402 | $1343.6 \cdot 10^{-8}$ | $1780 \cdot 10^{-8}$ | $0.3 \cdot 10^{-9}$ | 2.5 |
| 5 | Nitrogen dioxide | 46.0055 | 2.0527 | $829.72 \cdot 10^{-8}$ | $1112 \cdot 10^{-8}$ | $0.28 \cdot 10^{-9}$ | 2.5 |
| 6 | Water vapor | 18.01528 | 998.2 | $101.2 \cdot 10^{-8}$ | $101000 \cdot 10^{-8}$ | $0.29 \cdot 10^{-9}$ | 0.05 |

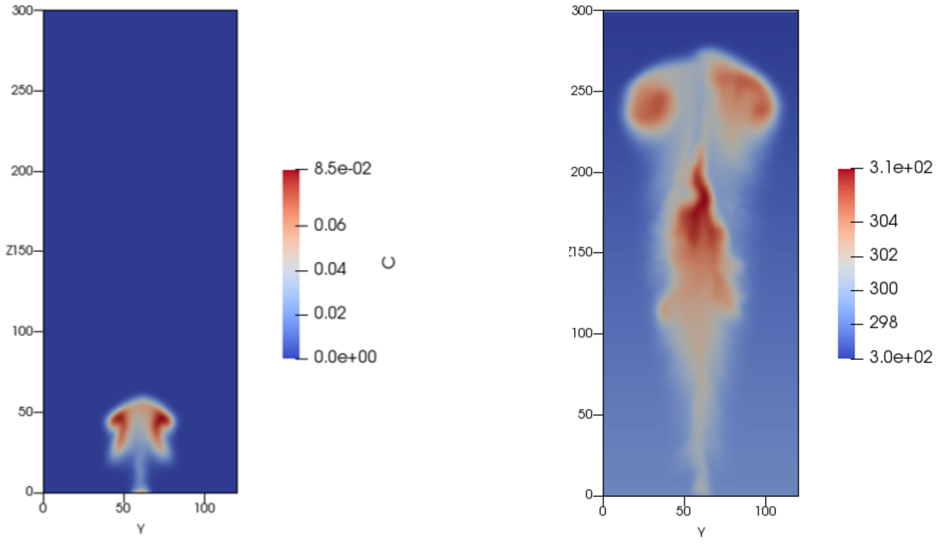
a) b)

**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 is observed on the upper part, 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 hot ball of heated air rises to the atmosphere until the temperature, the density of the external and internal heated and cold air's gas components equals, under the influence of buoyancy force. Effect of thermal radiation was not taken into account while performing numerical simulation. Fig.3 shows the dynamics of the concentration in the cloud. Fig.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.

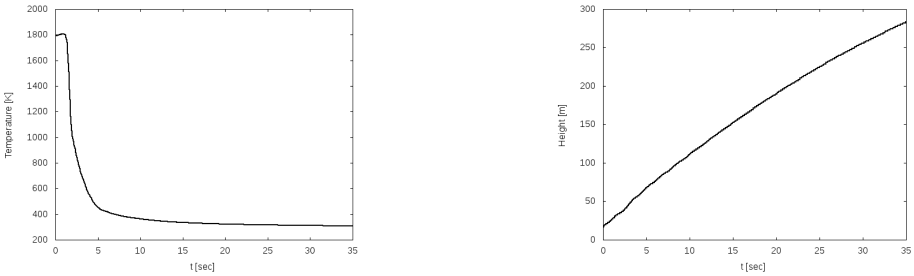
## Conclusion

There are obtained results of numerical simulation of cloud formation. There are determined cloud's geometric characteristics raised as a result of surfacing: height of the cloud, the cloud volume, and 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 Satton confirmed the applicability of the mathematical model used to the cloud formation problem in a surface explosion of a carrier rocket. The explosion power is calculated from the funnel size. The results of numerical simulation of cloud formation are obtained. The geometric characteristics of the cloud raised as a result of ascent are determined: the height of the cloud, the volume of the cloud, the shape of the vortex ring in the cloud. The blast power is calculated from the size of the crater. The obtained results of the simulation, which determines the height of the cloud elevation corresponds to the results of Onufriev [5], at low explosion power. 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



a) b)

**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 $x = 60m$: a) t = 5 sec; b) t = 35 sec.



a) b)

**Figure 4.** – Change of a) temperature; b) the formed cloud height with the explosion power q=0.878 ton.

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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