

NUMERICAL SIMULATION OF GASDYNAMIC PROCESSES AND THE DYNAMICS OF DUST PARTICLES IN CATASTROPHIC VOLCANIC EXPLOSIONS BY APPLYING TVD SCHEMES

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We developed a physicomathematical model to predict volcanic explosion-induced gasdynamic phenomena and the dynamics of the distribution of particles of ash and dust that precipitate onto the earth's surface and that remain in the atmosphere. We investigated the factors and processes that exert an influence on the transport of dust particles in the atmosphere. On the basis of the physicomathematical model developed, numerical simulation of volcanic explosions of specified power and space scale is done, and results on the dynamics of gasdynamic flows of air and the distribution of dust particles for different instants of time are analyzed.

Introduction. According to [1], volcanic eruption occurs due to accumulation of internal stresses in melted lava and its gas phase in the interior of the earth, resulting in a thermal explosion that breaks up the beds of rocks located above. Among the greatest historically known volcanic catastrophes by the volume of the material ejected, the ashfall area, and the energy of the explosion there are eruptions of the type of Santorin (1400 B.C.) and Tambora (1815) volcanoes. The characteristics of these explosions are the following [2]: the energy is estimated at the value 100 Gton, the volume of the material ejected is equal to about 50–185 km³, the ashfall area is about 1000 km². The repetition frequency of such catastrophes is one in about 10 thousand years. High-power eruptions markedly affect the earth's atmosphere, changing its gaseous composition and temperature and contaminating it with finely crushed material of volcanic ash, which is ejected into the upper layers and is then scattered by jet flows all over the globe. Consequently, it is of interest, from the viewpoint of reproduction of the observed parameters of such explosions and prediction of their dynamics and the consequences caused, to try to carry out numerical simulation of the phenomenon on the basis of the equations of gas dynamics.

1. Physical Model of a Volcanic Explosion. This model encompasses consideration of the process of formation and propagation of an explosion wave, the rise of an explosion cloud in the atmosphere, which contains dust particles, and the rise and precipitation of volcanic ash and dust particles. It is assumed that initially the entire energy of the explosion consists in the thermal energy of the gas contained in a hemispherical region on the earth's surface. At subsequent instants of time dispersion of the hot mass into an inhomogeneous atmosphere occurs. Most of the energy liberated as a result of the explosion is expended to form a shock wave, which propagates from the site of the explosion with a supersonic velocity and sets the surrounding air in motion and changes its pressure and temperature. The characteristics of the cold atmosphere (the distribution of the density and pressure with height) are determined with the aid of the model of the standard atmosphere CIRA-86 [3, 4].

The physical model of a volcanic explosion is based on separate description of the processes of dust transfer and development of the region disturbed by gasdynamic motion. The term dust in our model means a great variety of matter ejected from the volcanic neck. This matter can be characterized by exterior appearance (rocks, volcanic tuffs, pumice, ash, etc.), physical properties, chemical composition, and the distribution of mass. All this variety of matter is considered in the form of individual particles with a given discrete size distribution. It is assumed that the ejection of dust and the energy release occur instantly in the form of a single explosion. At the initial instant

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of time, a uniform distribution of the particles of dust is prescribed in the region of the energy release. The subsequent dynamics of these particles is described on the basis of the model of discrete representatives.

The model of formation and transfer of a dust cloud is based on three basic approximations. First, it is assumed that the dust particles move with a velocity equal to the local velocity of the air flow. This is valid for a wide range of sizes of particles, since the time in which the velocity of a dust particle attains the velocity of the entraining air flow has the order of several milliseconds. Second, reliable evaluations of the state of the dust medium can be made on the assumption that the gasdynamic fields are the same as in the absence of the dust. This assumption is valid if the kinetic energy of the dust particles is small in comparison with the total local energy of the air and its density is much smaller than the density of the air. Third, the motion of any dust particle or group of dust particles is independent of the presence or motion of any other particle or group of particles. This is valid if the number of dust particles per unit volume is not very large. In this case it is possible to consider each group of particles separately, and the characteristics of the entire dust cloud can be obtained by summing up the corresponding characteristics of all the groups.

Transfer of dust particles occurs due to gasdynamic motion of air masses and due to local turbulent motion. In the vertical direction the dust particles also experience the action of the gravitational force, which causes the dust cloud to descend. The influence of thermal effects on the dust is neglected in the present model. The given model of cold dust can be used for both intermediate and later instants of time. It also allows one to evaluate the relative effect of certain assumptions and coefficients that are associated with the description of formation and transfer of a dust cloud.

2. Mathematical Model. The mathematical model used to describe the evolution of a volcanic explosion in the atmosphere is based on gasdynamic differential equations that express mass, momentum, and energy conservation laws. They can be expressed mathematically in Eulerian variables in the following form:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} &= 0, \\ \frac{\partial \rho u}{\partial t} + \frac{\partial (p + \rho u^2)}{\partial x} + \frac{\partial \rho uv}{\partial y} + \frac{\partial \rho uw}{\partial z} &= \rho g, \\ \frac{\partial \rho v}{\partial t} + \frac{\partial \rho uv}{\partial x} + \frac{\partial (p + \rho v^2)}{\partial y} + \frac{\partial \rho vw}{\partial z} &= 0, \\ \frac{\partial \rho w}{\partial t} + \frac{\partial \rho uw}{\partial x} + \frac{\partial \rho vw}{\partial y} + \frac{\partial (p + \rho w^2)}{\partial z} &= 0, \\ \frac{\partial e}{\partial t} + \frac{\partial u(p + e)}{\partial x} + \frac{\partial v(p + e)}{\partial y} + \frac{\partial w(p + e)}{\partial z} &= \rho gu. \end{aligned}$$

The total energy is associated with the remaining quantities by the relation

$$e = \rho I + \frac{1}{2} \rho (u^2 + v^2 + w^2).$$

In the case of a perfect gas $I = p / [\rho(\gamma - 1)]$, where $\gamma \approx 1.4$. This system of gasdynamic equations is solved by using the numerical method of finite differences [5], the essence of which consists in replacement of a continuous medium by some discrete model of it. Here the physical space is approximated by a difference grid, and the differential equations of gas dynamics that describe the initial problem are approximated by a system of algebraic equations. The process of evolution of gasdynamic characteristics is traced from some initial instant of time through a number of finite increments on a set of discrete cells.

To carry out a difference approximation of the system of gasdynamic equations over space, an explicit TVD scheme [6] of second order of accuracy is used. To pass from the n -th to the $n + 1$ -th time layer, a two-stage Runge–Kutta TVD scheme [7] is used, which also has second order of approximation in time. The TVD schemes

belong to the class of ENO schemes [8]. In these schemes, automatic transformation of the kinetic energy of a shock wave front into thermal energy is provided and generation of nonphysical oscillations along shock waves is absent. The latter is attained due to an automatic mechanism of feedback to control the amount of numerical dissipation. Generally, TVD schemes make it possible to resolve shock waves within 2–4 cells. An advantage of theirs is the fact that they provide the possibility of investigating, with good accuracy, gasdynamic flows whose velocity is much lower than the characteristic speed of sound. This is especially important in simulation of the motion of a dust cloud at the last instants of time, when the velocity of air motion becomes small (10–20 m/sec) and the state of the dust cloud is determined by the parameters of the circulating air flows.

The problem is considered in a rectangular Cartesian coordinate system. It is assumed that the x_1 axis is directed upward, the x_2 axis to the right, and the x_3 axis is perpendicular to the plane (x_1, x_2) . The plane (x_2, x_3) corresponds to the surface of the earth. The half-space $x_1 > 0$ is occupied by the atmosphere. The source of energy release is located in the plane (x_2, x_3) and in the upper half-space $x_1 > 0$. The processes occurring in the dense medium ($x_1 < 0$) are not considered.

The calculation of the gasdynamic characteristics is done on a nonuniform grid whose dimensions are determined by the region of the air disturbed by the motion. When the air flow reaches one of the boundaries of the grid, the cells of the grid are enlarged according to a geometric progression with a specified coefficient. Thus, the evolution of the gasdynamic motion of air masses is traced over greatly changing space and time scales.

At the initial instant of time, in a hemispherical region of a certain radius that is adjacent to the air-ground interface ($x_1 = 0$) the initial energy release (which corresponds to a certain temperature) is prescribed at the background value of the density. The coefficient of compression of the region of energy release along the vertical axis is used. All the remaining cells of the spatial grid are filled with background values of the parameters of the atmosphere. The condition of zero leakage is set as the boundary conditions on the surface $x_1 = 0$. The upper and side boundaries of the computational domain are free. They are expanded as the region disturbed by the motion develops.

3. Model of Particles-Representatives. To describe the motion and interaction of the dust particles with the surrounding air flow the following model is used [9]. Volcanic ash is considered to be a polydisperse system of particles of prescribed mass. The aggregate of particles that are localized in some region of space and have nearly the same characteristics is represented in the form of a single particle-representative with properties that are characteristic for the given set of particles. The mass of the representative is taken equal to the total mass of the entire aggregate of particles. The state of each particle-representative is determined by specifying the following parameters: three spatial coordinates, three components of velocity, and mass, which are needed to describe motion in the space of the aggregate of identical particles corresponding to the particle-representative.

To simulate the motion of particles-representatives in a cloud, the Monte Carlo method is used. It is assumed that each representative is entrained by the air flow at the point of space at which it is located with the local gasdynamic velocity of the air V . Moreover, it moves relative to the air under the force of gravity. Thus, a particle of diameter 0.1 mm falling under gravity in air of normal density acquires its final velocity in 0.1 sec. Therefore one can try to take into account the influence of gravitation on the motion of a representative in terms of its final velocity v_p , which depends on the size of the particle and local gasdynamic characteristics of the air at the point of space at which it is located. The expression that describes the dependence of the absolute value of the final velocity of a particle, acquired by the latter under the action of the gravitational force, on its characteristics and the local parameters of the air can be represented in the form [9]

$$v_p = \sqrt{\left(\left(\frac{24\mu}{\rho d_p} \right)^2 + \frac{8}{3} \left(\frac{\rho_p}{\rho} \right) g d_p \right) - \frac{24\mu}{\rho d_p}}.$$

The ash and dust particles ejected by a volcano also ascend due to the process of air turbulization. To take this phenomenon into account, a semiempirical coefficient of diffusion is introduced:

$$A = 0.2s^2 / (1 + (s/V)^2) \quad [\text{m}^2/\text{sec}],$$

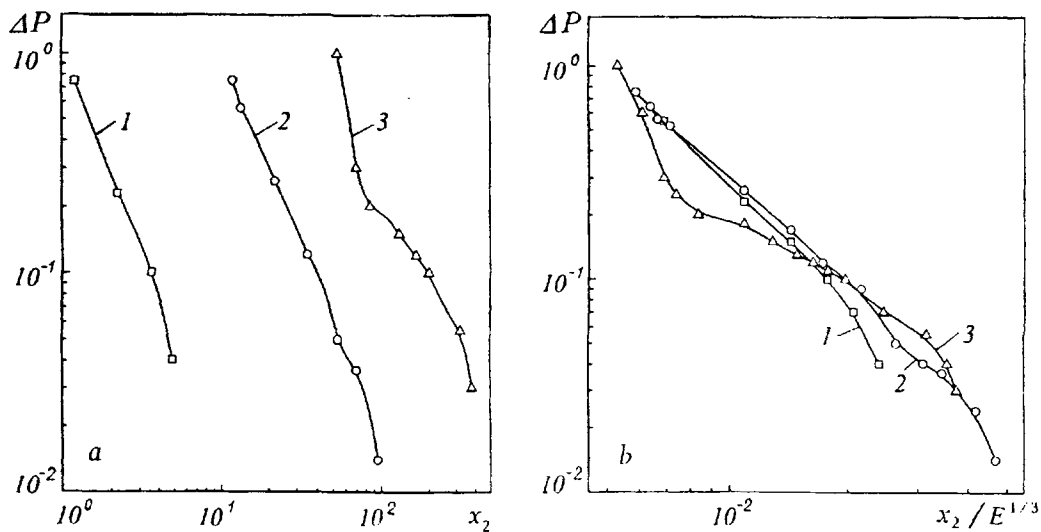


Fig. 1. Dependence of the excess pressure of the shock wave front on the distance (a) and the dimensionless radius (b): 1) $E = 0.8$, $R = 1$; 2) 800 and 10; 3) 10^4 and 50. ΔP , atm; x_2 , R, km; E , Mton.

where $s = 300$ m/sec. Taking into consideration all the effects indicated above, it is possible to determine the motion in space of any particle-representative within a rather short interval of time Δt by means of the following expression:

$$\Delta r = (V + v_p) \Delta t + n \sqrt{6\Lambda \Delta t}.$$

While moving, each particle-representative intersects the cells of the computational gasdynamic grid. If a particle-representative intersects the boundary that corresponds to the surface of the earth, the falling-out of dust particles is fixed. As a result, for each instant of time the distributions of dust particles in space and the density of their mass can be obtained.

The total mass of an ejection is one of the most indeterminate characteristics. It depends in the main on the composition of the substance ejected. The quality of the description of the cloud of an ejection by the model of discrete representatives is determined by the way the ejected mass is spread over the particles-representatives. The size distribution of the ash and dust particles is associated with the properties of the material ejected and can vary in a wide range. In the present model it is described by a lognormal law with a constant dispersion and median. The mass function of the representatives in relation to the diameter has the form

$$\Phi(d_p) = \frac{6 \cdot 10^3}{\pi \rho_p} \frac{\exp(4.5\sigma^2)}{\xi^2} \frac{1}{\sqrt{2\pi} \sigma d_p} \exp\left(-\frac{1}{2} \left(\frac{\ln d_p}{\sigma \xi_p}\right)^2\right), \quad 1/g \cdot \text{mm},$$

where ρ_p is given in g/cm^3 , $\xi_p = \xi \exp(-3\sigma^2)$ in mm, and d_p in mm.

4. Results of Numerical Simulation. On the basis of the above physicomathematical model of a volcanic explosion the three-dimensional computer code VEDEM (Volcano Eruption and Dust Environment Modeling) was developed in the FORTRAN-90 language. The aim of this code is to predict the development of the region of the explosion and the dust loading of the atmosphere. The VEDEM code makes it possible to carry out in a three-dimensional geometry a numerical experiment on simulating a single explosion with a specified energy release and radius. Using this code, simulation of a series of problems concerning the explosion of a volcano with different powers was done with account taken of ejection of dust.

Simulation of the problem of the explosion of a volcano is considered in the following formulation. At the initial instant of time it is assumed that the entire energy release is contained in the thermal energy of gas that has a certain temperature and density and occupies a hemispherical volume of specified radius. Along the height the radius of the region of energy release decreases by a factor of three. At subsequent instants of time the expansion of the hot region into an inhomogeneous atmosphere is considered. To describe dust particles in the

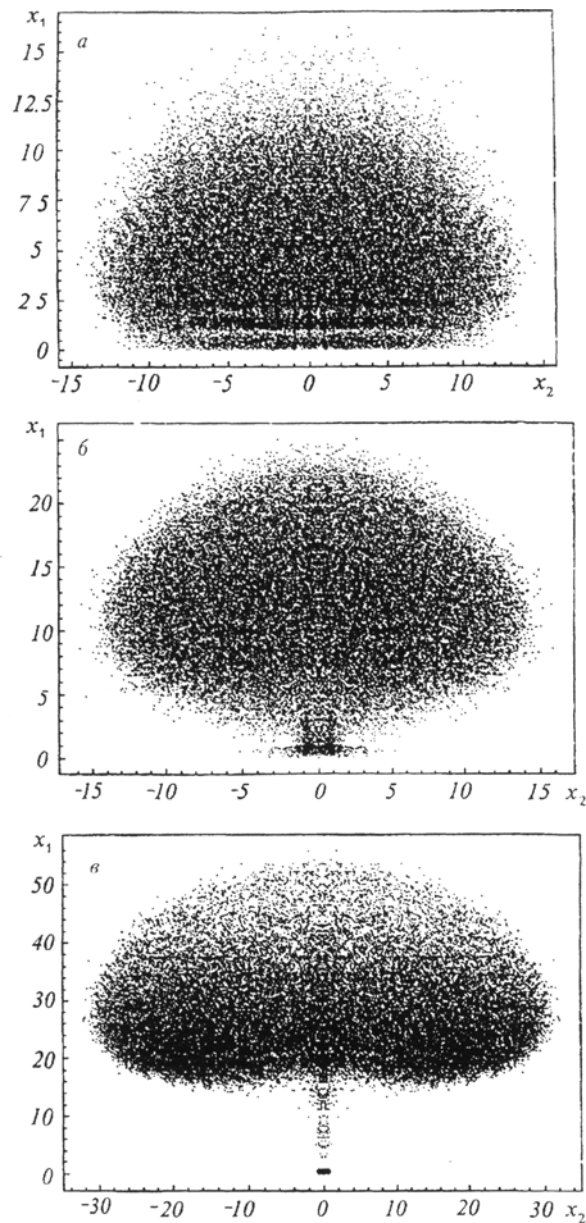


Fig. 2. Dynamics of the formation of a dust cloud [a) 51.16 sec; b) 1.69 min; c) 3.69 min]. View along the x_3 axis. The initial characteristics of the explosion of a volcano: $E = 800$; $R = 10$. The proportion of the mass of dust present in the air: a) 90.35; b) 89.55; c) 89.46%. The percentage distribution of the mass of dust for each of 15 discrete diameters d_p (0.27; 0.5; 0.93; 1.7; 3.2; 5.9; 11; 20; 37; 68 μm ; 0.13; 0.23; 0.43; 0.8; 1.5 mm) is the following: a) 1.76; 2.84; 4.17; 5.75; 7.35; 8.86; 9.73; 10.15; 9.82; 8.68; 7.29; 5.63; 4.06; 2.64; 1.62%; b) 1.75; 2.81; 4.15; 5.72; 7.33; 8.82; 9.69; 10.06; 9.72; 8.63; 7.23; 5.56; 3.97; 2.55; 1.55%; c) 1.75; 2.81; 4.15; 5.72; 7.33; 8.82; 9.69; 10.06; 9.72; 8.64; 7.23; 5.56; 3.96; 2.52; 1.49%. x_1 , km.

diameter range from 0.2 μm to 2 mm 15 discrete sizes of particles (groups) were used. The number of particles-representatives in each of the groups was specified to be equal to 3000.

In order to investigate the development of the gasdynamic region and formation and transfer of the dust cloud in relation to the power of the explosion, simulation of the following three variants with initial conditions was done: the radius of the explosion 1, 10, and 50 km, the value of the energy release in the hemisphere 80 kton, 800 Mton, and 100 Gton. The mass of the dust ejected is the most indeterminate value, and it depends on the

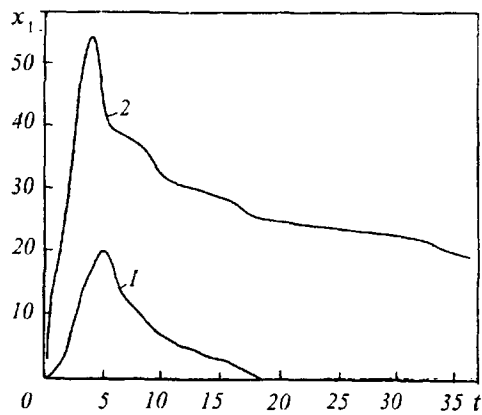


Fig. 3. Variation of the height of the lower and upper boundaries of a dust cloud with time: 1) lower and 2) upper boundaries of the dust cloud. t , min.

composition of the volcanic matter. Therefore, it was arbitrarily taken equal to unity. Determination of the mass of the ejection in this way is possible, since in our model the inverse effect of the dust particles on the gasdynamic air flow is ignored. The radius and the magnitude of the energy release were specified proceeding from the condition that the initial temperature in the region of the explosion be equal to approximately 1700 K. Since the problem is symmetric about the vertical axis, only the region of space that is limited to one of the quadrants was considered.

The dependence of the back pressure on the distance along the surface of the earth for the three variants considered is presented in Fig. 1a. It is known [10, 11] that an excess pressure of the order of 0.05–0.07 atm leads to damage to ground-level objects. As is seen from the figure, damage will be caused at a radius of about 4.5, 55, and 350 km. The shock wave that moves along the surface of the earth attains these distances by instants of time of 10 sec, 2.2 min, and 7 min, respectively. Figure 1b illustrates the dependence of the back pressure on the dimensionless radius defined as the ratio of the distance to the cube root of the total energy. From the theory of a point explosion it follows that for different energy releases the motion of the shock wave front must possess similarity properties. From specified characteristics of one explosion, it is possible to determine the parameters of explosions with other initial energies by means of simple conversion. For any assemblage of such explosions all the corresponding dimensionless characteristics must have identical numerical values. Despite the fact that in each of the variants a different size of the initial region of energy release was specified, satisfactory coincidence of the calculated curves is observed at distances that are severalfold larger than the region of energy release, showing the closeness of the calculations and the results of point-explosion theory.

As a result of numerical simulation, the dependence of the formation and transfer of a dust cloud in the atmosphere on the value of the initial energy release was investigated. Calculations for the three variants were carried out up to a time of about 30 min from the beginning of the explosion. As an example, Fig. 2 presents results on the dynamics of formation of a dust cloud for an explosion with a radius of 10 km and an energy release of 800 Mton. The primary growth and formation of the dust cloud are completed in a very short period of time equal to about 1 min (Fig. 2a). Due to the formation of a rarefied volume and its rise in the region of the explosion, complex vortical motion of the air appears, which exerts a direct effect on the rise and formation of the dust cloud. The number of particles in the lower portion of the cloud decreases with time (Fig. 2a), since the particles are entrained in the wake of the ascending rarefied region. By a time of about 1.7 min the dust cloud separates from the surface of the earth and ascends to 25 km (Fig. 2b). The number of particles in the upper portion of the cloud decreases with time under the force of gravity. The dust begins to concentrate near the lower boundary (Fig. 2c). By a time of about 3.7 min the size of the dust cloud attains a radius of more than 30 km due to the action of horizontal air flows (Fig. 2c). At a later stage, large particles of dust that initially were raised by strong air flows to a considerable height precipitate in the atmosphere. Thus, by a time of about 18 min intense precipitation of such particles onto the surface of the earth begins. This is illustrated by Fig. 3, which shows the time dependence of the height of the lower and upper boundaries of the dust cloud. Thus, at later instants of time the dust cloud consists in the main of small-sized particles, with separation of groups of dust particles with different diameters occurring over height. This is evident from Fig. 4. By a time equal to 35.19 min dust particles with diameters from 0.27 to 68 μm are

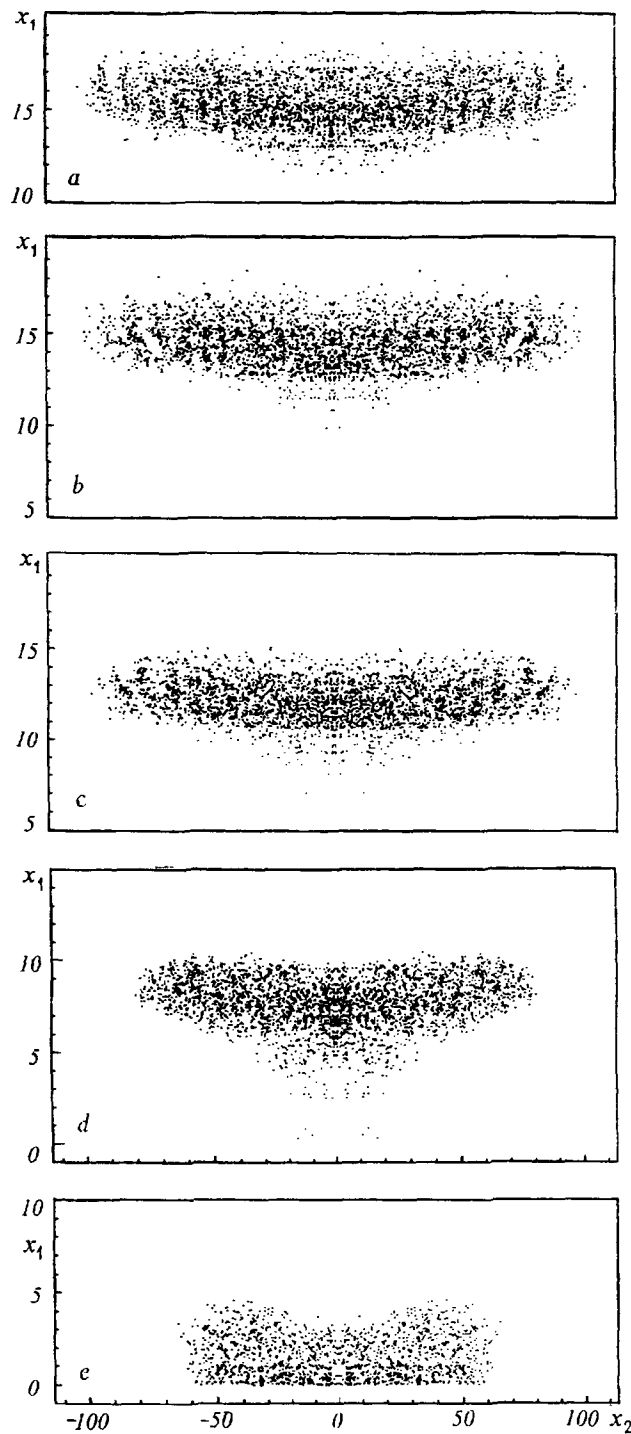


Fig. 4. Distribution of groups of particles of different diameters d_p over height: [a) $0.69 \mu\text{m}$; b) 0.13 ; c) 0.23 ; d) 0.43 ; e) 0.8 mm] at a time of 35.19 min. The proportion of the mass of dust present in the air is 86.49%. The percentage distribution of the mass of dust over the groups is the following: a) 8.63; b) 7.21; c) 5.52; d) 3.91; e) 1.24%. The group of particles having a diameter of 1.5 mm entirely falls out of the cloud onto the surface of the earth.

found at a height of more than 15 km. As an example, Fig. 4a shows a group of particles with a diameter of $68 \mu\text{m}$. The distribution over height of groups of dust particles with diameters from 0.13 to 0.8 mm is presented in Fig. 4b-e. By this time, the group of particles with a diameter of 1.5 mm has precipitated entirely from the cloud. This separation is associated with the discrete description of the diameters of the dust particles. With an increase in the number of groups, a continuous size distribution of the particles over height will be observed. However, this leads

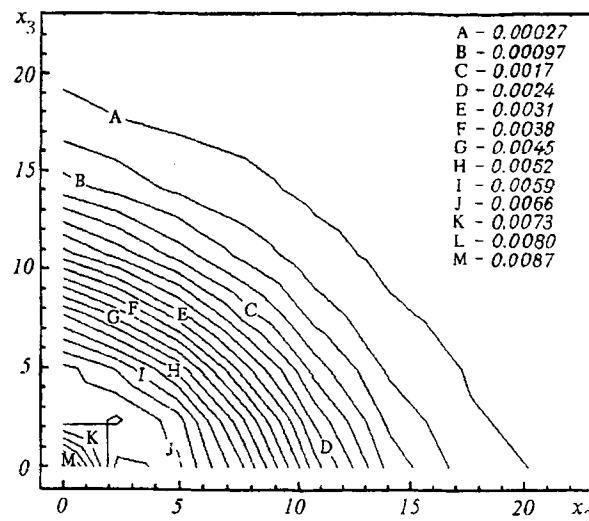


Fig. 5. Distribution of the precipitated mass of dust over the surface of the earth: $t = 35.19$; $E = 800$; $R = 10$. The proportion of the mass of dust that fell out onto the surface of the earth is equal to 13.51%. The scale determines the relative fraction of mass per unit area ($1/\text{km}^2$). x_2, x_3 , km; t , min.

to an increase in the amount of computation and in the expenditure of machine time. The distribution of the precipitated mass of dust over the area is presented in Fig. 5. It is seen that by a time of about 30 min the area of dust precipitation is more than twice the area of the initial ejection. The main mass of dust precipitates within the radius of the explosion. The scale on the figure determines the distribution of the relative mass of dust (normalized to the total mass of the dust precipitated) over the area.

The above-described model of gas dynamics on TVD schemes was used to test numerical simulation of an explosion of a volcano and the dynamics of the dust cloud in a three-dimensional Cartesian coordinate system, in spite of the fact that the problem studied has cylindrical symmetry. This serves as a good test for the described three-dimensional code VEDEM and gives the possibility of subsequently investigating truly three-dimensional problems associated, for example, with a horizontal wind. The results of the conducted investigation for the three variants presented demonstrate the possibilities of the model developed. However, to establish the similarity and characteristic features of the formation and dynamics of a dust cloud it is necessary, in the case of volcanic explosions of high power and large radius, to carry out calculations up to substantially longer times than was done in the present investigation. This is associated with the fact that the time scale of the evolution of air flows for such explosions is much larger than for low-power ones. The difficulty in tracing the dynamics of a dust cloud up to appreciable times is associated with substantial expenditures of computing time, which are outside our computer possibilities.

The model of gas dynamics on TVD schemes is very time-consuming and requires large expenditures of machine time, especially for the case of three-dimensional calculations. Thus, for example, using a $50 \times 30 \times 30$ spatial grid and an explicit TVD scheme that has first order of accuracy in time and second in space, the expenditures of machine time to calculate one time step on a Pentium-II-266 computer is approximately 2 min. To trace the dynamics of a dust cloud to a time of the order of 1–2 h, calculation of more than 5000 steps is required. When the Runge–Kutta scheme is used, which has second order of approximation in time, the expenditures of computing time to calculate a time step increase by a factor of two.

The physicomathematical model presented above to describe three-dimensional gasdynamic flows on the basis of TVD schemes is more accurate and informative than the two-dimensional axisymmetric model of the method of "large particles" developed earlier [12, 13]. In the present model the use of TVD schemes allows suppression of the onset of nonphysical oscillations of velocity, and this makes it possible to apply it to describe the gasdynamic motion of air at late instants of time. This model describes rather accurately weak gasdynamic flows that have a velocity of about 10–20 m/sec. In the method of large particles, at these velocities oscillations of

the velocity of the gasdynamic flow that have no physical meaning appear. At large times a consequence of this is vertical and horizontal wavy oscillation of the dust cloud.

Conclusion. The above physicomathematical model makes it possible to carry out a numerical experiment on simulation of explosion phenomena in an inhomogeneous atmosphere, such as the impact of a meteorite against the surface of the earth and the explosion of a volcano, and to predict their consequences. The results of the simulation make it possible to follow in time the dynamics of the development of the explosion region and the formation and transfer of the dust cloud and to obtain the distribution of the precipitated dust over the area. In the model presented a volcanic eruption is considered in the form of a single instantaneous explosion with a prescribed energy release and radius. However, in reality a volcanic eruption is a more complex phenomenon. A volcanic explosion is a particular case of eruption that causes the most catastrophic consequences. Other types of eruption are also of interest for simulation, and, consequently, further refinement of the model is required. This modification can be made in the following directions:

1. Taking into account the duration of the eruption, i.e., consideration of a sequence of several noninstantaneous explosions of different power separated in time. The difficulty consists in correct description of subsequent ejections, since by a given instant of time the spatial region disturbed by the first explosion can reach substantial scales.

2. Simulation of a directed jet ejection of volcanic gas and dust into the atmosphere with a prescribed duration and rate of discharge.

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NOTATION

x_1, x_2, x_3 , axes of the Cartesian coordinate system; t , time; x, y, z , spatial coordinates in the Cartesian system; \mathbf{V} , vector of gasdynamic velocity; u, v, w , components of the vector of gasdynamic velocity in Cartesian coordinates; ρ , density; p , pressure; e , total energy; g , free-fall acceleration directed opposite to the x_1 axis; I , specific internal energy; γ , specific-heat ratio; μ , viscosity of air; d_p , diameter of a dust particle; ρ_p , density of the substance of a dust particle; \mathbf{v}_p , vector of the final velocity of a dust particle; A , coefficient of diffusion; \mathbf{n} , random unit vector uniformly distributed in space; Δr , motion of a dust particle; Δt , time step; σ , dispersion; ξ , median; R , radius of the explosion; E , initial energy release; ΔP , excess pressure; s , constant. Subscript: p, particle.

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