High Temperature, Vol. 37, No. 6, 1999, pp. 873–879. Translated from Teplofizika Vysokikh Temperatur, Vol. 37, No. 6, 1999, pp. 904–911.
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HEAT AND MASS TRANSFER AND PHYSICAL GASDYNAMICS

Numerical Simulation of the Processes of Propagation of Impurity from a Large-Scale Source in the Atmosphere

A. V. Konyukhov, M. V. Meshcheryakov, and S. V. Utyuzhnikov

Moscow Physicotechnical Institute, Dolgoprudnyi, Moscow oblast, 141700 Russia

Received July 2, 1998

Abstract—The structure of convective columns forming during a fire is investigated numerically. The maximum height of a convective column and the height of spread for different values of energy release and size of the site of fire are determined. The dependence of the results on constants in the algebraic model of turbulence is analyzed. The calculation results are compared with the data of laboratory experiments. Model calculations are performed in a three-dimensional formulation.

INTRODUCTION

During the last decade, efforts of a number of authors went into the construction of a mathematical model of a large-scale fire, primarily, of a city fire. In the monograph [1], the main causes of emergence of such fires are investigated and classified, and a definition is given of a large-scale fire which is different from an ordinary industrial (or forest) fire by the high intensity of combustion and/or by the rate of development. In the monograph [2], possible consequences of fires for the global climate due to the emission into the atmosphere of aerosol particles in the form of soot and ash are discussed. Estimates are given of reserves of "potential fuel" for such fire and of the mass of smoke under different conditions of combustion. The monograph [3] is devoted to various aspects of simulation of forest fires. In [4–6], calculation models were proposed based on the set of Navier–Stokes equations with constant transport coefficients. In further studies [7–9], different versions of algebraic models of turbulence were used. In [10], the observation data on the fire in Hamburg are given, as well as the results of its numerical simulation, in which the real values of energy release during a city fire are included. The latter paper also contains the data on the oil fire in Long Beach (1958), which was treated as a point source at the radius of 0.5 km. In numerical and laboratory experiments [9, 11], it was shown that formulas for a point source are invalid for the calculation of the heights of hovering and spread of a convective column with the radius of the site of fire greater than 8 km. And the site of such fire cannot be treated as a point source.

This study is devoted to more detailed investigation of this problem. Namely, the defining parameters of numerical and laboratory experiments (in particular, the value of energy release in the site of fire) are made more consistent in a wide range. Calculations are performed with different values of the constant in the formula for the mixing length $K = 0.125$ (borrowed from [7, 8]), $K = 0.2$ [10], and $K = 0.4$. A comparison of the results of laboratory experiments and calculations reveals that the best coincidence is observed for the case of $K = 0.2$. Possibilities are discussed of using differential models of turbulence in calculations based on the procedure proposed and used by us in [12–14]. As was shown previously in [8], phase transitions caused by the presence of moisture in the atmosphere influence strongly the parameters of lift, hovering, and transport of aerosol to the atmosphere. In this study (as in [9]), these effects were not taken into account. This is explained, on the one hand, by the fact that it was necessary to study the basic regularities of flow using the model of dry atmosphere and, on the other hand, by the fact that the calculations were correlated with the data of a laboratory experiment, in which the humidity of the atmosphere was not taken into account, rather than of a full-scale one.

Note that the treated physical phenomenon of large-scale fire is characterized by a number of important singularities, which are not reproduced if two-dimensional (plane or axisymmetric) models are used. In this study, some results are given of calculations of the site of fire in a three-dimensional formulation (including the case of side wind), which have not been performed until now. This is associated with high requirements placed by the problem on the resolution of the algorithm both in the neighborhood of the site of fire and in the regions of convective rising flow and the region of hovering and spread of a convective column.

FORMULATION OF THE PROBLEM

In this study, we treat a set of equations of turbulent motion of compressible gas, written with respect to the quantities averaged according to Favre [15] (except for

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the density and pressure), and complemented by the algebraic model of turbulence [9],

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0,$$

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot (\rho \mathbf{V}\mathbf{V} + p\mathbf{I} - \mathbf{R}) = \rho \mathbf{g},$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left(\rho \mathbf{V}\left(E + \frac{p}{\rho}\right) - \mathbf{R} \cdot \mathbf{V} + \mathbf{q}\right) = \rho \mathbf{g} \cdot \mathbf{V}.$$

The equations are closed on the basis of the Boussinesq approximation, according to which the Reynolds stress tensor is proportional to the tensor of average deformation rates,

$$\mathbf{R} = -\frac{2}{3}\mu_t \nabla \mathbf{V} \mathbf{I} + 2\mu_t \mathbf{S},$$

where $\mathbf{R}$ is the Reynolds stress tensor, S is the tensor of deformation rates, and $\mathbf{I}$ is the unit tensor, as well as by the relation for the heat flux

$$\mathbf{q} = -\frac{\mu_t}{\sigma_t}\nabla e, \quad \sigma_t = 0.9.$$

The equation of state $p = (\gamma - 1)\rho e$ with the adiabatic exponent $\gamma = 1.4$ is used. The cylindrical system of coordinates (r, φ, z) is used; the plane $z = 0$ corresponds to the earth surface, and the z-axis is directed vertically.

The values of the coefficients of turbulent transport were calculated using the algebraic model of [9] (it was also used in [7, 8]), according to which, in the axially symmetric case, the turbulent viscosity μ_t is defined by the formulas

$$\mu_t = \frac{\rho l^2}{2}\left\{\left(\frac{\partial v}{\partial z} + \frac{\partial u}{\partial r}\right)^2 + 2\left[\left(\frac{\partial v}{\partial r}\right)^2 + \left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{v}{r}\right)^2\right]\right\}^{1/2},$$

$$l = K\left\{(v^2 + u^2)^{1/2}B^{-1/2} + B^{1/2}\left[\left(\frac{\partial^2 v}{\partial r^2} + \frac{1}{r}\frac{\partial v}{\partial r} - \frac{v}{r^2}\right)^2 + \left(\frac{\partial^2 v}{\partial z^2}\right)^2 + \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r}\right)^2 + \left(\frac{\partial^2 u}{\partial z^2}\right)^2\right]^{-1/2}\right\},$$

$$B = \left(\frac{\partial v}{\partial r}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2 + \left(\frac{v}{r}\right)^2 + \left(\frac{\partial u}{\partial r}\right)^2 + \left(\frac{\partial u}{\partial z}\right)^2,$$

in which l is the mixing length and K is the empirical constant. In numerical calculations, it was assumed that $\mathrm{Pr} = 1$, and the value of K was varied. (Note that the coefficient of dynamic viscosity μ_l is omitted in the set of equations, because the relation $\mu_t \gg \mu_l$ holds for the problem at hand.)

Similar to [9], the diffusion equation for the impurity concentration was not treated. The impurity was modeled by the introduction of a certain number of particles on the external side of the site of fire in fixed time intervals and by the calculation of motion of such particles on the basis of kinematic equations of motion (for details, see [13]). It was revealed in previous studies that such an approximation of a "passive" impurity makes it possible to describe fairly adequately the distribution of emissions of smoke and aerosol during a large-scale fire.

In the (r, z) plane, the calculation region is a rectangle with the dimensions $2R_0$ (in r) and $H = 24$ km (in z). A standard atmosphere is used in the calculations [9]. At the initial instant $t = 0$, the static pressure is assumed to be equal to the atmospheric pressure at the height z above the sea level in the entire calculation region. The source of energy release was preassigned in the form of a cylinder of radius R_0 and height h equal to 100 m. The volume source intensity Q^* varied in time following the linear law to the value of $Q^*_{\max}$, which was reached in 30 min, as in [5, 7, 8]. After that, the intensity of the source was assumed to be constant. Note that the variation of the time during which the source reached the maximum power $(0 < t^* < 30)$ showed that the heights of hovering and spread of a convective column are almost independent of this time.

NUMERICAL PROCEDURE

The calculation was performed using the TVD scheme of the second or third (for three-dimensional formulation) order of approximation in space variables (except for the extreme points of characteristic variables) and of the first order in time for the Eulerian part of equations [14]. For the approximation of processes of diffusive transfer, a scheme of the first order in time and of the second order in space was used.

The employed method of linearization of the hyperbolic part of equations [15] provided the three-diagonal structure of the block matrix of coefficients, corresponding to each coordinate direction. In the calculation of the Jacobi matrices–flow vectors of the Reynolds part of equations (Reynolds stresses, heat fluxes, and dissipative function), only the differentiation operators which contributed to the principal diagonal of the coefficient matrix were linearized; in so doing, the viscosity coefficients were taken from the lower time layer.

To reduce the bulk of calculations in the solution of the linearized set of equations, at each time step the method of approximate factorization was used, which consists in representing the operator on the left-hand side of equations in the form of the product of two one-dimensional operators.

The sets of algebraic equations obtained as a result of factorization of the operator on the left-hand side of

Table 1

<table>
<tr><td colspan="7">The value of energy release in the site of fire $Q = 0.073$ MW/m^2</td></tr>
<tr><td colspan="2">$R_0 = 5$ km</td><td colspan="4">$R_0 = 12$ km</td><td>$R_0 = 22$ km</td></tr>
<tr><td>$K = 0.125$</td><td>$K = 0.2$</td><td>$K = 0$</td><td>$K = 0.125$</td><td>$K = 0.2$</td><td>$K = 0.4$</td><td>$K = 0.2$</td></tr>
<tr><td colspan="7">The value of energy release in the site of fire $Q = 0.24$ MW/m^2, $K = 0.2$</td></tr>
<tr><td>$R_0 = 1$ km</td><td colspan="2">$R_0 = 2$ km</td><td>$R_0 = 5$ km</td><td colspan="2">$R_0 = 12$ km</td><td>$R_0 = 22$ km</td></tr>
</table>

equations, which had a block three-diagonal matrix, were solved using the vector sweep method.

In the axisymmetric formulation, calculations were performed on a stationary 81×121 net with the maximum Courant number of 0.75 in the flow field. The Courant number is restricted by the accuracy requirement; the calculations indicate that its further increase results in a fast increase of the dissipative error of the scheme. The net was concentrated toward the earth surface and toward the z-axis. Namely, the calculation region was divided in four parts: in the site of fire, a uniform 40×6 net was preassigned; above the site, a 40×115 net uniform in r and expanding in z to a preassigned value of the upper boundary; on the right of the site, a 40×6 net uniform in z and expanding in r to the value of the outer boundary; on the right of the site and above it, a 40×115 net expanding in r and z. In the three-dimensional formulation, the finite-difference net contained $50 \times 50 \times 100$ nodes. In calculations, the boundary conditions were preassigned similar to [9]. The accuracy of such calculations was monitored by the mass and energy balance. In addition, calculations were performed on nets with different numbers of nodes, with the dimensions of the net given above selected from the considerations of calculation accuracy and independence of the calculation results of preassignment of the outer boundaries.

Calculations were performed on a Pentium Pro 150 personal computer (32 MB RAM). The time required for the calculation of 1 h of physical time was about 30 h (for axisymmetric formulation).

CALCULATION RESULTS

One of the main objectives of this study was to reach a good agreement between the calculation and available experimental data [14, 15]. This would define the limits of validity of algebraic models of turbulence and the need for transition to differential models. In view of this, calculations were performed for different values of preassigned empirical constant in the formula for the mixing length, which enters the employed algebraic model. It was previously shown that the calculation results in the problem on floating of a single thermal in a stratified atmosphere [12] depend significantly on the value of this constant. Table 1 gives the values of defining parameters of the problem, which were varied during calculations.

The preassigned values of energy release were in agreement with the data of laboratory experiments [14, 15] and with the data of other authors. Thus, $Q = 0.23$ MW/m^2 at a lower value of $t^* = 300$ s [6], and $Q = 0.05$ MW/m^2 at $t^* = 1800$ s [5, 8]; in [5], the cases $Q = 0.1$ MW/m^2 and $Q = 0.025$ MW/m^2 were also treated. The latter value of $t^* = 1800$ s agrees well with the estimates of time during which the maximum of energy release in a large city fire is reached. At the same time, it is clear that the value of $Q = 0.05$ MW/m^2 corresponding to the complete combustion of wood materials with the area density of load of 10 kg/m^2 for one hour (at the calorific power of fuel $Q_0 = 19.6 \times 10^6$ J/kg) is underestimated for a large city fire. According to the data on the fire in Hamburg in July 1943 [10], one can estimate the power at 1.7×10^6 MW with the surface area of 12 km^2. This gives the power of the source $Q = 0.14$ MW/m^2 with the site radius $R \simeq 2$ km. Note further that, according to the same data, the wind was weak at the instant of the emergence of fire, and the humidity of the atmosphere was low. The values of other parameters were also close to those adopted in the simulation: the tropopause was at the level of 11.5 km, the temperature in stratosphere was 216 K, and the temperature at the ground was 288.1 K. The observation results were as follows: the height of the smoke column was 12 km, and the region of maximum smoke concentration several hours after the commencement of fire was 8–9 km. These data are in good agreement with the calculation results of [10]. In addition, the maximum vertical velocity of convective flow of 68 m/s was obtained in the calculations.

We will treat the main stages of simulated gasdynamic flow. Note that the initial stage of formation of flow is physically close to the problem on surface thermal [12]. On the periphery of the site of fire, a wall flow begins to develop directed toward the site region. With time, this flow is transformed into a vortex. In contrast to the case of surface thermal, where such a vortex covered the entire region of flow, a much more complex pattern is observed in the treated problem. Due to the large size of the site of fire (not less than 5 km), a peripheral vortex does not have enough time to move to the axis region, where a vortex of its own is formed; at first, it is less developed than the peripheral one, but then it develops quickly, and it is the axis vortex that is then transformed to a convective column. A similar flow pattern was revealed in [9]. It was also established

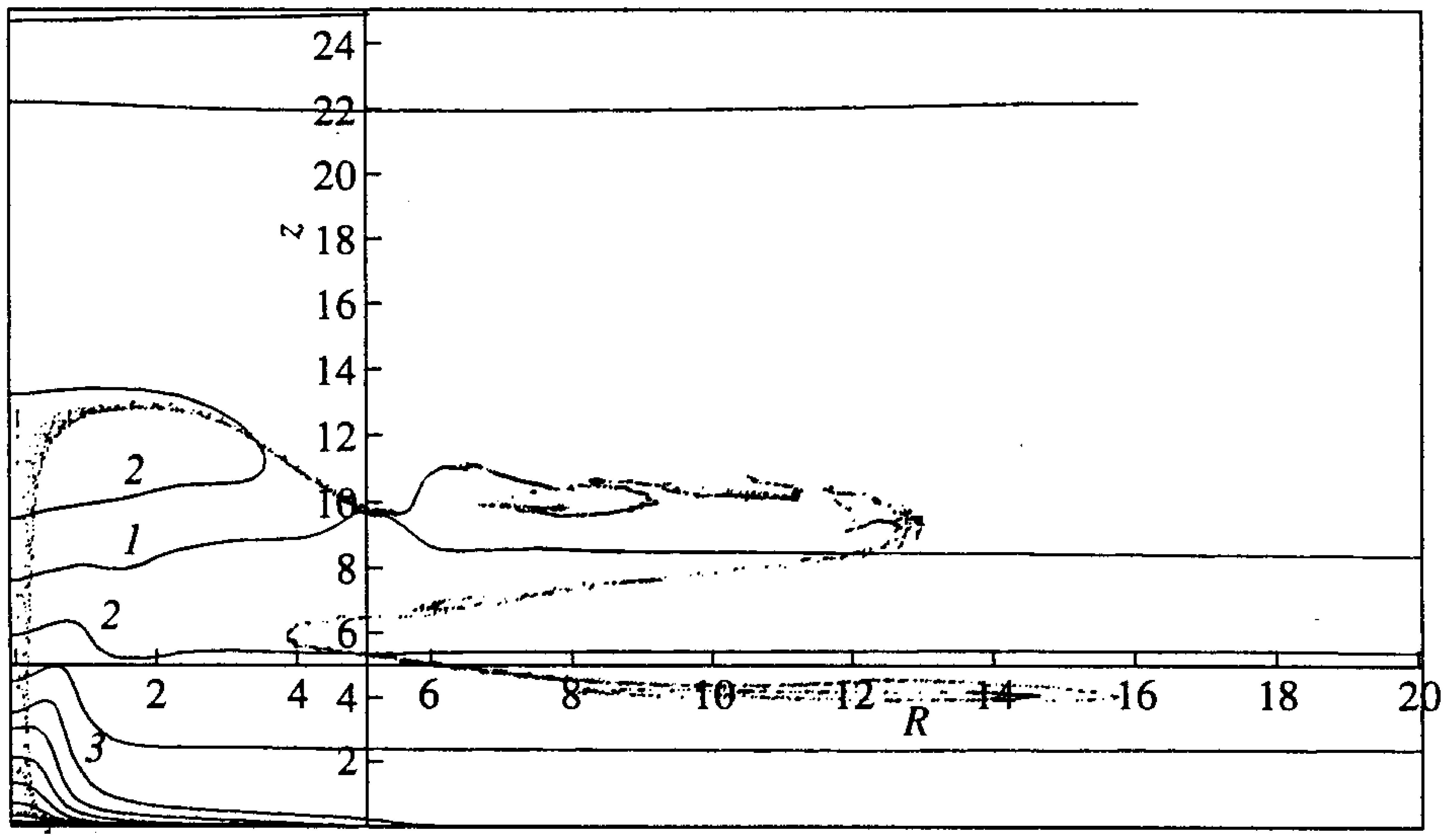

Fig. 1. Temperature isolines (solid curves) and the field of impurity distribution for R_0 = 5 km and Q = 0.24 MW/m^2 and the instant t = 60 min. Isoline (*1*) indicates T = 230 K, (*2*) T = 250 K, (*3*) T = 270 K, and so on, with ΔT = 20 K (T_{max} = 430 K).

there that, with the radius of the site of fire exceeding 10 km (i.e., the characteristic height of the tropopause $H^* \simeq$ 11 km for middle latitudes), the initial stage of flow is even more complex and characterized by the presence of more than two vortexes. It is such a multivortex cellular structure of fire with a radius of more than 10 km that results in the absorption by complex vortex flows of a considerable part of the energy released during the fire. Consequently, the formation of a convective column is slowed down, and the heights of hovering and spread of the convective column are lower at the late stage of flow development.

The calculation results for K = 0.2 and the data of laboratory experiment transformed to the form convenient for comparison are given in Table 2. Here, H_{max} is the height of hovering; H^* is the height of spread of the convective column; h_{max} and h^* are the heights of hovering and spread, respectively, recalculated from the laboratory experiment using the similarity theory [11]. The table gives averaged values of the height of hovering of the top edge for the time interval t = 30–60 min, because the top edge oscillates about its equilibrium position.

Table 2

R, km	Q, MW/m^2	H_{max}, km	h_{max}, km	H^*, km	h^*, km
5	0.073	8.3	8.3	5.1	5.3
12	0.073	11.2	9.7	6.0	5.2
22	0.073	12.0	11.8	6.0	5.6
5	0.24	12.1	13.4	8.0	9.3
12	0.24	17.2	16.5	11.0	9.5
22	0.24	18.8	18.7	10.5	9.7

As is seen in Table 2, the calculation data and the data of laboratory experiment are in satisfactory agreement. Nevertheless, although the calculations made it possible to select the constant K = 0.2 in the algebraic model, which provided good agreement with laboratory experiment, by and large, such an approach leaves room for discussion. (If the value of K = 0.125 was preassigned in the calculations, we obtained values which exceeded the experimental data by 30–35% and, with K = 0.4, values 40–50% less than the experimental data.) The main problem associated with the use of algebraic models is that they are not capable of describing complex effects associated with significant curvature of the lines of current and with high vorticity. However, numerous foreign and Russian researchers used versions of algebraic models in such calculations without an analysis of their effect on the obtained solution. Therefore, this study was devoted to a detailed analysis of one of the widely used algebraic models. In so doing, one parameter of the model was varied, and comparison was made with the results of laboratory experiment. The main conclusion is that one can select a suitable parameter for the model after testing this model with experimental data. Then, calculations of the impurity propagation will have an acceptable error level for different technological processes [16]. For a fundamental treatment of the problem at hand, differential models of turbulence must be involved. Up to now, these models were not used in calculations of large-scale fires. Problems associated with the use of models of this type will be addressed in future investigations. At the level of technological estimates of propagation of impurities, one can restrict oneself to simpler approaches. Below, all calculation data are given for the versions with K = 0.2, or another value of K is given.

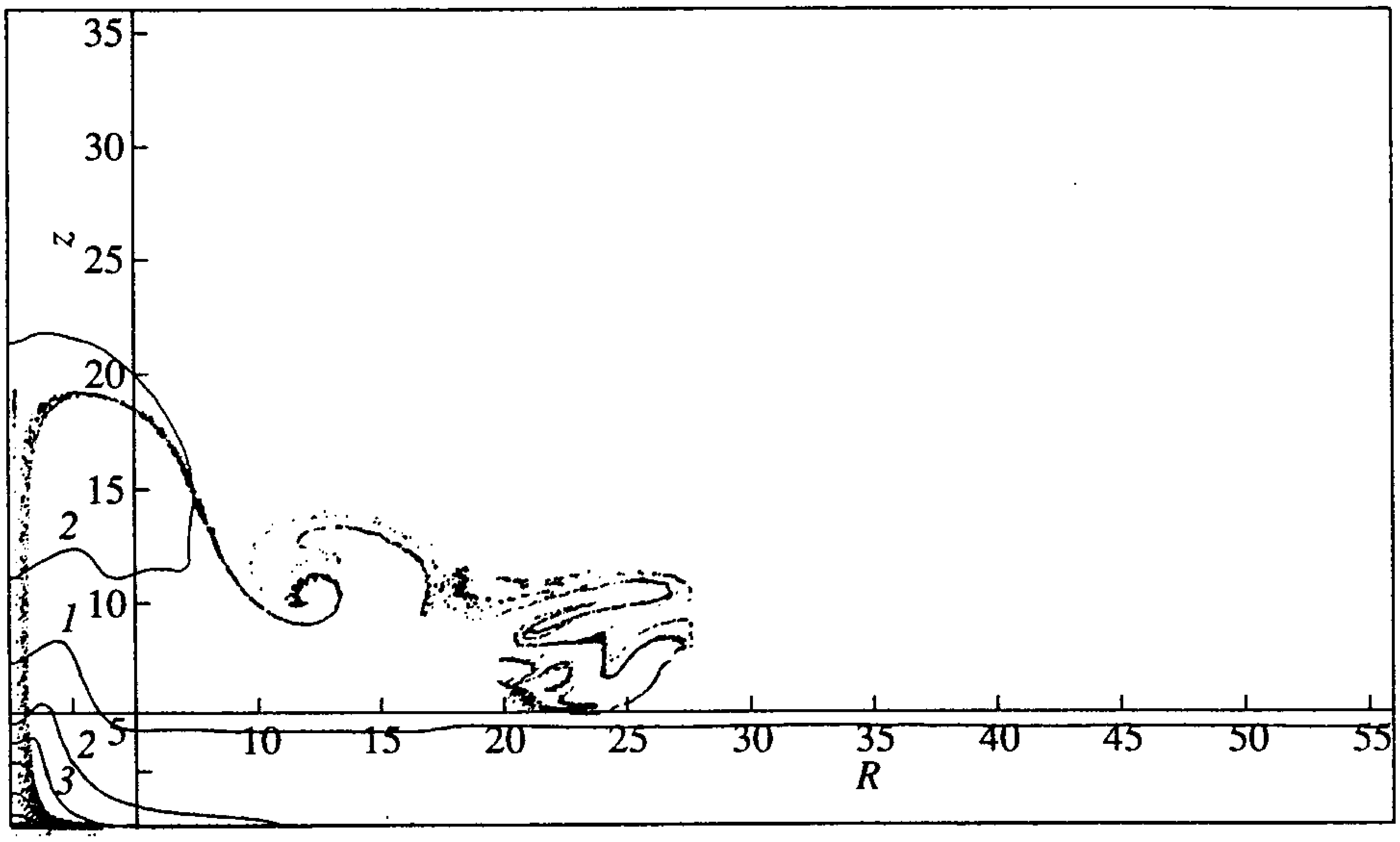

Fig. 2. Temperature isolines (solid curves) and the field of impurity distribution for the version of $R_0 = 12$ km and $Q = 0.24$ MW/m^2 at the instant $t = 40$ min. Isoline (*1*) indicates $T = 255$ K, (*2*) $T = 305$ K, (*3*) $T = 355$ K, and so on, with $\Delta T = 50$ K ($T_{max} = 720$ K).

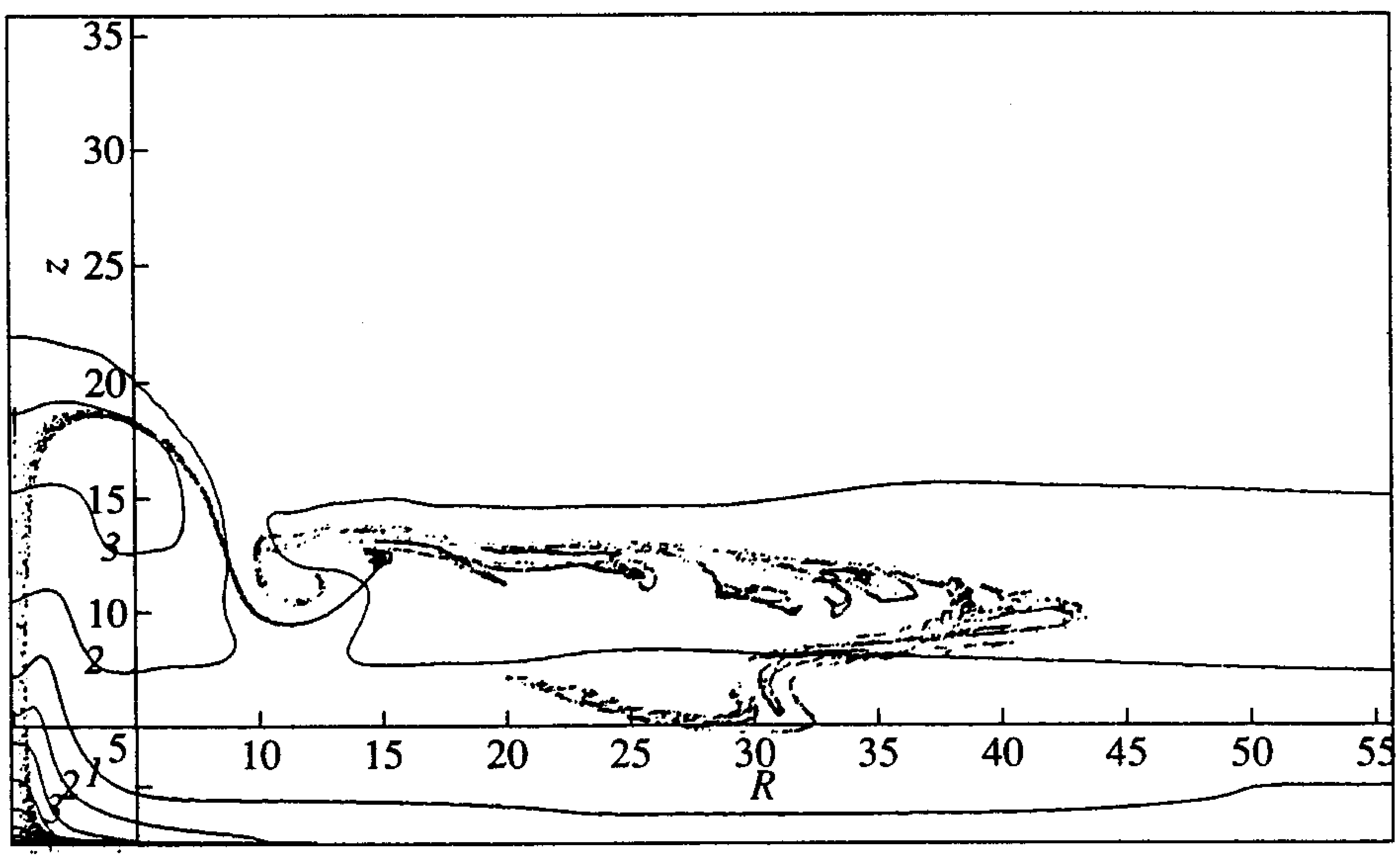

Fig. 3. Data similar to those of Fig. 2 for the instant $t = 60$ min, $R_0 = 12$ km, and $Q = 0.24$ MW/m^2. Isoline (*1*) indicates $T = 260$ K, (*2*) $T = 285$ K, (*3*) $T = 310$ K, and so on, with $\Delta T = 25$ K ($T_{max} = 650$ K).

Figure 1 gives the temperature isolines and the field of impurity distribution for the version with the site radius $R_0 = 5$ km and $Q = 0.24$ MW/m^2 at the instant $t = 60$ min. The pattern is characteristic of the stage of hovering of a convective column and spread of the tongue of impurity cloud.

Figure 2 gives the temperature isolines and the field of impurity distribution for the version with $R_0 = 12$ km and $Q = 0.24$ MW/m^2 at the instant $t = 40$ min. It is seen that the convective column has already reached the height of hovering, although the temperature in its front part is still higher than the temperature of the environment. In the region of the tongue of impurity, complex vortex structures are clearly seen. Figure 3 gives the instant $t = 60$ min for the version with $R_0 = 12$ km and $Q = 0.24$ MW/m^2, for which the quasistationary form of impurity distribution is characteristic. For the sake of comparison with Fig. 2, Fig. 4 gives the form of convective column for $R_0 = 12$ km, $Q = 0.073$ MW/m^2, and $t = 40$ min for the case of $K = 0$ (disregarding the effect of turbulence).

The effect of the side wind on the parameters of a convective column, in particular, on the height of removal of a passive impurity from the site of fire to the

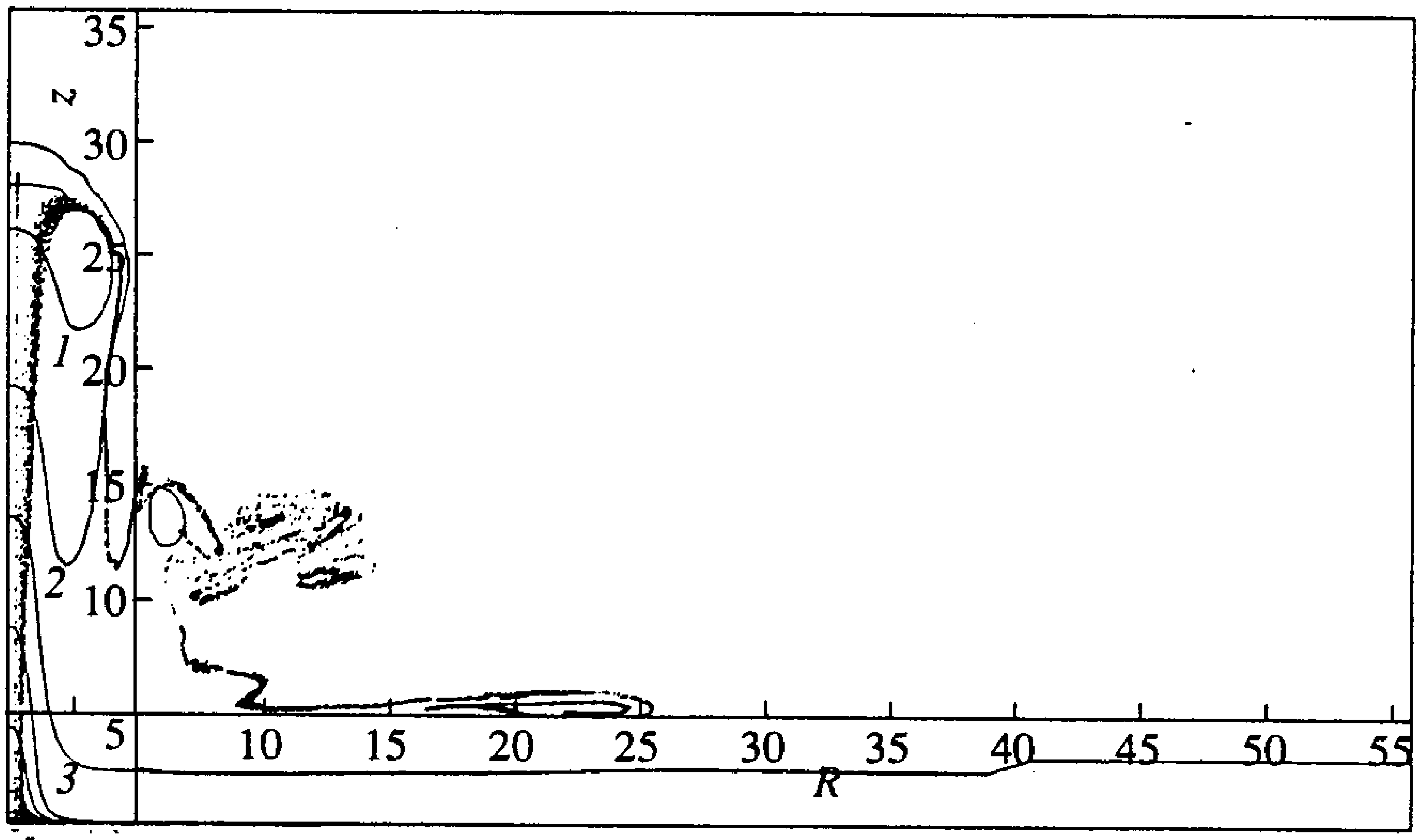

Fig. 4. Data similar to those of Fig. 2 for the version of R_0 = 12 km and Q = 0.073 MW/m^2 corresponding to the instant t = 40 min obtained assuming the absence of the effect of turbulence (nonviscous calculation). Isoline (*1*) indicates T = 200 K, (*2*) T = 235 K, (*3*) T = 270 K, and so on, with ΔT = 35 K (T_{max} = 550 K).

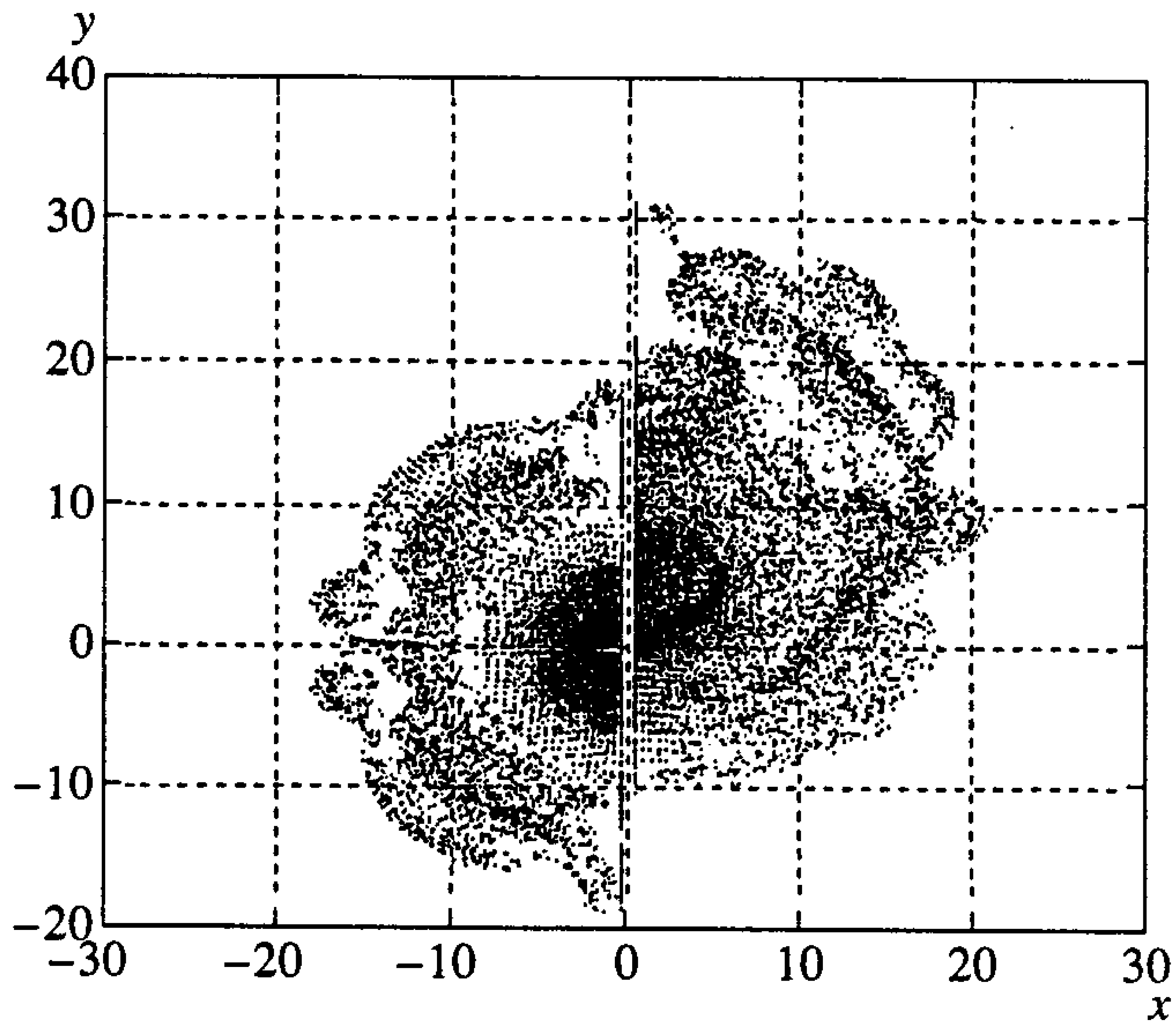

Fig. 5. Projection of impurity cloud (top view) at t = 20 min without (on the left) and with the wind (on the right), R_0 = 10 km and Q = 0.05 MW/m^2 (the velocity of the side wind is 10 m/s, and the direction is indicated by the arrow in the figure). Designations on the axes is given in km. Dot (0, 0) corresponds to the epicenter of fire.

atmosphere, was investigated. A simple model of the site of fire in the form of a spatial source (of energy and impurity) of cylindrical shape and with energy release constant in volume and time was used in the calculations.

The initial parameters of the problem were as follows: the site radius R_0 = 10 km, the source power Q = 0.05 MW/m^2, and the wind velocity was 10 m/s (stratification of the wind in height was not given). Equations of motion for nonviscous gas were integrated using the MUSCL TVD scheme [17], which had the third order of approximation in space variables and the second order in time.

The initial stage is characterized by the formation of a toroidal vortex on the periphery of the site of fire. After 15 minutes, an intense rise of heated gas and propagation of a cloud in the radial direction at a height of the order of 4.5 km take place in the region above the source.

The visualization of flow was performed by introduction of a source of passive impurity in the site of fire. Figure 5 gives projections of a cloud (top view)

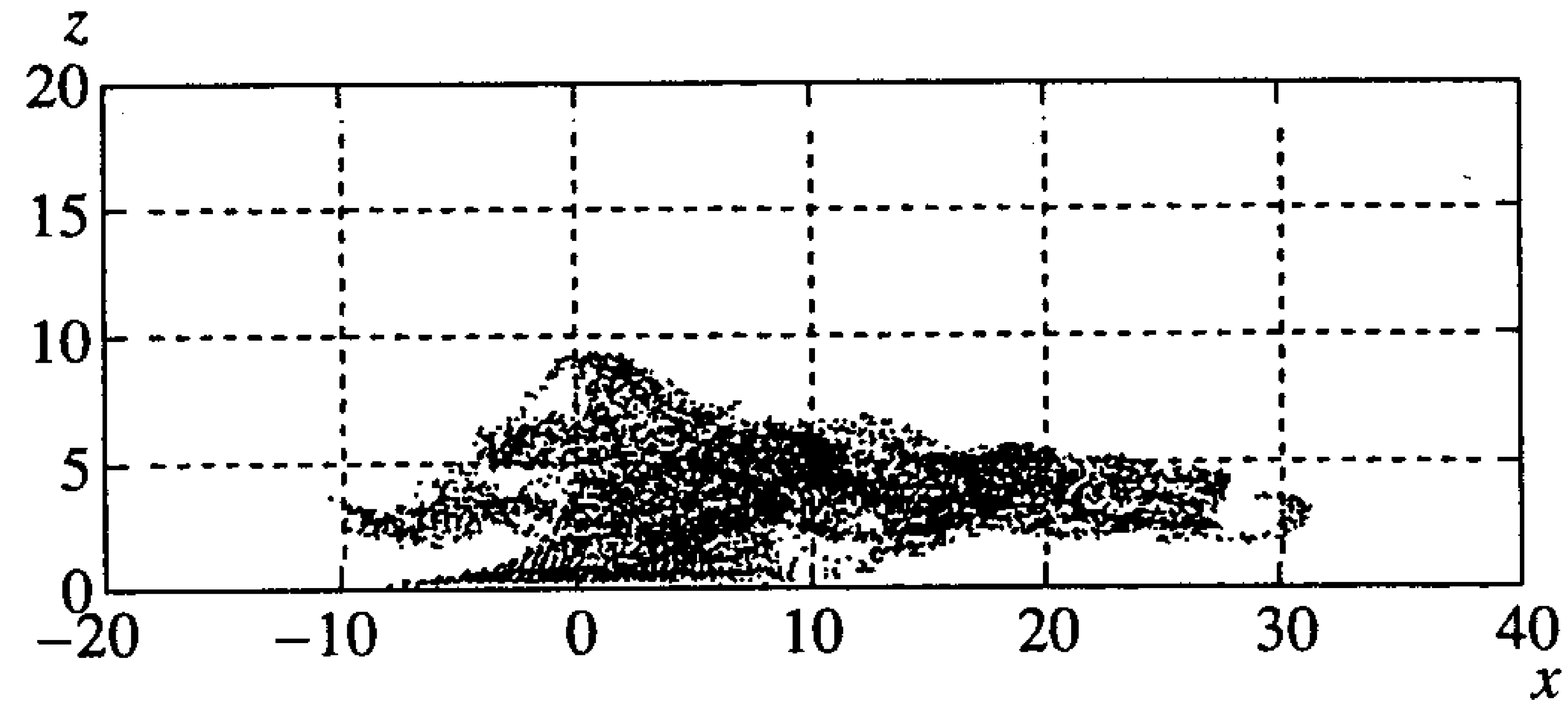

Fig. 6. Side view of the site of fire (in the xz-plane) with the wind (its direction coincides with the $0x$-axis) for the same calculation and time as in Fig. 5.

above the site of fire at $t = 20$ min without (on the left-hand side) and with the wind (on the right-hand side). The direction of wind is indicated by the arrow. Note that, although the source of fire is a figure of revolution (in the absence of wind, the distributed impurity is not one). This is indicative of the instability of an axisymmetric solution of this problem. Figure 6 gives the side view for the same instant in the presence of wind (it is directed from left to right). The axes in both figures are marked in kilometers.

Note that these calculations were treated as a first step for the transition to investigation of this problem in a three-dimensional formulation. Therefore, in the three-dimensional case, one can so far talk only about the qualitative structure of flow rather than about concrete quantitative results. A complete model must allow for the turbulent characteristics of gas motion, the diffusion equation for impurity transport, and wind stratification in height.

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