POLLUTION OF THE ATMOSPHERE BY FIRE AND EXPLOSION THERMALS

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ABSTRACT

Mathematical model of a large-scale dusty thermal in a stratified non-uniform atmosphere is presented, which takes into account the compressibility of atmosphere and active effect of pollutant on the motion of carrier gas. An entrainment of various pollutants by a rising thermal is investigated, a final distribution of particulate matter density formed in atmosphere after rise of the thermal is obtained. Quantitative boundaries of applicability of a wide-spread model of "passive" impurity are established.

KEYWORDS: Convection, Thermal, Explosion, Pollution, Modeling.

INTRODUCTION

In recent years more and more attention is paid to possible ecological consequences of large fires and explosions. For example, much attention is focused on global ecological and climatic consequences of massive pollution of upper atmosphere with optically active aerosol particles entrained by powerful convective flows.[1,2]

The so-called convective elements may have been formed in the atmosphere as a result of quasi-continuous (plumes) or instantaneous (thermals) energy release from fires or explosions. Large quantities of earth material, dust, soot, ash etc. can become involved in the fireball gases, especially for a surface high-yield burst, which can have a marked effect on the fireball early-stage evolution. A greate deal of such particulate and gaseous pollutants will then be carried aloft with the rising fireball and injected into the upper troposphere and lower stratosphere, while some large fragments will rain out of the cloud to form a close-in fallout.[3]

In this paper some aspects of numerical modeling of pollution of atmosphere by rising gaseous and dusty turbulent thermals are considered.

MATHEMATICAL MODEL

Consider a spherical hot gaseous cloud (fireball or thermal) located initially above the flat horizontal surface. Suppose that this cloud contains some particulate or gaseous pollutant distributed over its volume. Introduce a cylindrical coordinate system (r, z) by placing its origin onto the surface beneath the centre of the thermal. The time-dependent evolution of such a thermal is governed by the following set of equations with initial and boundary conditions:

$$\frac{\partial \rho}{\partial t} + \rho(\nabla\vec{U}) = 0, \quad P = \rho_1 T, \quad \rho = \rho_1 + \rho_2 \qquad (1)$$

$$\rho\frac{d\vec{U}}{dt} = -\frac{1}{\gamma M^2}\nabla P + \frac{1}{Re}[\Delta\vec{U} + \frac{1}{3}\nabla(\nabla\vec{U})] - \rho\vec{j} \qquad (2)$$

$$(\rho_1 + \gamma_1\rho_2)\frac{dT}{dt} = -(\gamma-1)P(\nabla\vec{U}) + \frac{\gamma}{RePr}\Delta T \qquad (3)$$

$$\frac{\partial \rho C}{\partial t} + \nabla(\rho C\vec{U}) = \frac{1}{ReSc}\Delta C, \qquad C = \frac{\rho_2}{\rho} \tag{4}$$

$$t = 0: \quad \vec{U} = 0, \quad T = T_a + \theta_o \exp[(-(r^2+(z-H)^2)/R^2] \tag{5}$$

$$P = P_a, \quad \rho_2 = M_{21}\exp[-(r^2+(z-H)^2)/R^2]$$

$$r = 0: \quad u = 0, \quad \partial(v, P, T, C)/\partial r = 0 \tag{6}$$

$$z = 0: \quad \vec{U}=0, \quad \partial T/\partial z = \partial C/\partial z = 0$$

$$r^2 + z^2 \to \infty: \quad \vec{U} = 0, \quad T = T_a, \quad P = P_a, \quad C = 0$$

Here, the subscripts 1 and 2 relate to the gaseous and disperse phases, $\vec{U} = (u, v)$ - velocity, ρ - density, P - pressure, T - temperature, $\vec{j}$ - vertical unity vector, C - concentration of pollutant. The Eq. (1) - (6) are reduced to non-dimensional form using parameters P_0, T_0 and ρ_0 of the gas in undisturbed atmosphere near the surface as reference values. The length scale has been set to a certain fixed value L of the order of typical initial radius of the thermal; the velocity and time scales are then $(Lg)^{1/2}$ and $(L/g)^{1/2}$ respectively. The results are presented below in a form of relationships that do not depend on specific value of L. In Eq. (1)-(6) $\gamma_1 = C_2/C_V$ is the phase specific heats ratio, M_{21} and θ_0 determine the loading and excess temperature of the cloud, R and H - initial radius and height of the thermal. Parameters of undisturbed atmosphere T_a, P_a, ρ_a are described by the model of standard atmosphere. In non-dimensional form temperature and pressure distributions are expressed as

$$\frac{1}{T_a}[\frac{dT_a}{dz} + (\gamma-1)M^2] = k, \quad \frac{dP_a}{dz} = -\gamma M^2 \rho_a, \quad \rho_a = \frac{P_a}{T_a} \tag{7}$$

where $k = N^2L/g$ - stratification parameter. Up to the tropopause ($z < H_T = H_T^o/L$, H_T^o = 10 - 16 km) $N^2 = 1.2 \cdot 10^{-4}\ s^{-2}$, above - $N^2 = 4.4 \cdot 10^{-4}\ s^{-2}$. The corresponding non-dimensional stratification parameters are denoted hereafter as k_1 ($z < H_T$) and k_2 ($z > H_T$). The Navier-Stokes equations are used here because the vertical scale of convective flows considered is large enough, so that the variation of atmospheric density with height owing to the compressibility of the gas is significant. Under these conditions the use of more simple models of incompressible fluid, i.e., of those basing on the Boussinesq approximation, is not valid. The Eq. (1) - (6) were solved numerically by a three-layer extrapolating finite-difference scheme using the alternating direction implicit (ADI) algorithm.[4] Non-uniform (refining near the axis and underlying surface) 40 x 50 adaptive grids were used to integrate the equations. A program **TERMAX** (**ThERMal AXi**symmetric) was written in FORTRAN 77 and intended for VAX 11/780 computer; besides, an IBM PC/AT 386/387 - oriented version of this code is available which provides an interactive menu-driven input and graphics screen output.

GASEOUS THERMAL

To close the system of governing equations (1) - (6) a proper method for selecting the values of turbulent transport coefficients (i.e., of Re and Pr criteria) should be implemented. An approach basing on calculation of the self-similar coordinate of the cloud top is used here. It can be outlined as follows.

Analysis of experimental data on dynamics of ascent of turbulent thermals[5] shows that at the self-similar stage of evolution the vertical coordinate of a foremost part of the thermal Z_t increases according to the law

$$Z_t - Z_o \approx 4.35\, I_o^{1/4} t^{1/2}, \qquad I_o = \frac{Q_o}{2\pi \rho_o C_p T_o L^3} \tag{7}$$

where Z_0 is the virtual origin, Q_0 - heat of formation of the thermal (for nuclear bursts Q_0 is approximately equal to 35% of the total yield). The most remarkable feature of this relationship is that the self-similar coordinate of the cloud top $\xi_t = (dZ_t/dt^{1/2})\, I_o^{-1/4}$ is roughly constant in very wide range of thermal energy Q_0 and takes a value of $\xi_t \approx 4.35$. To make use of (7) in determining the turbulent transport coefficients calculations were made for $\gamma = 1.4$, $M = 0.3$, $Re = 20 - 100$, $Pr = 1$, $H = 1.56 - 7.42$, $\theta_o = 5 - 21$, $I_0 = 0.34 - 2.71$, $k = k_1 = 1.2 \cdot 10^{-2}$. These parameters correspond to fireballs of explosions with yield $W = 2.1 - 16.7$ MJ ($L = 10^3$ m, $T_0 = 273$ K, $P_0 = 1$ bar). If the parameters of atmosphere are taken to be constant, the dependence of self-similar coordinate on the four principal parameters H, θ_0, I_0, Re can be reduced to the dependence on just two values: the first of them $H' = \gamma M^2 H$ is the ratio of initial cloud height to the scale of atmospheric density variation $1/\gamma M^2$, the second one is a modified Grashof number $Gr = Re^2 I_0$. This dependence may be factored into the product of two functions each depending on a single parameter:

$$\xi_t(H, \theta_o, I_o, Re) = \xi_t(H', Gr) = F(H') \cdot G(Gr) \tag{8}$$

$$F(H') \approx P_a(H'), \qquad G(Gr) \approx 4.92\left(1 - \frac{252}{Gr + 346}\right), \quad 100 \le Gr \le 2000$$

where the approximating formulas were found as a best fit to results of calculations.

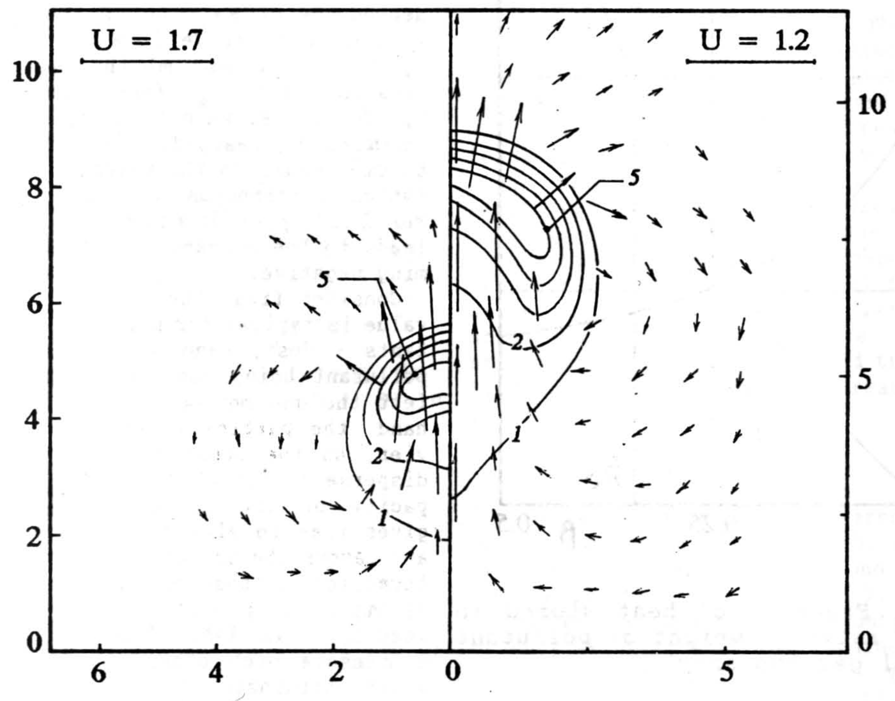


Fig. 1. Excess temperature contours within the turbulent thermal: left - t = 2.8, right - t = 8.7. Velocity field is shown by arrows.

Thus, given an initial heat energy of the thermal and its height, Grashof number can be readily obtained from (8) by equating ξ_t to experimental value 4.35. This method enables us to determine the turbulent transport coefficients that guarantee a valid ascent velocity of the thermal at the self-similar stage of the ascent, which is supported by comparison of calculated and experimental cloud heights at different moments.

In Fig. 1 two sequential moments of the gaseous thermal ascent are presented: on the left $t = 2.8$ (initial stage), on the right - $t = 8.7$ (self-similar ascent). Isotherms 1 - 5 correspond to excess temperatures $\theta = 0.2, 0.4, 0.6, 0.8, 1.0$ (left) and $\theta \cdot 10 = 0.22, 0.44, 0.66, 0.88, 1.1$ (right). Velocity field is shown by arrows in both sides of Fig. 1. Penetration of the thermal into the stratosphere is followed by intensive cooling of the gas resulting in inversion of temperature field: at the moment of maximum ascent the gas in the thermal is supercooled with respect to surrounding atmosphere. Initial toroidal vortex is replaced by this time by a system of two counter-rotating vortices. A complex multi-vortex flow field structure features the oscillations of the thermal at the final stage of evolution.[6]

PARTICULATE THERMAL

In presence of disperse pollutant within the cloud bulk the initial heat energy of the thermal becomes distributed over the gaseous and particulate phases: $I_0 = I_g + I_p$. Two parameters feature the initial thermal and force effects of pollutant: $\beta = C_2 M_0 T_0 / Q_0 = \gamma_1 m / 2\pi\gamma I_o$ (M_0 - total mass of pollutant, m - its dimensionless value), $\alpha = F_- / F_+$ ($F_- = m$ - non-dimensional weight of dust, $F_+ = 2\pi I_o$ - total gas buoyancy). The fraction of heat energy stored in gas $\sigma_g = I_g / I_0$ in a broad range of m, γ_1 and I_0 depends just on a single parameter β. This dependence is shown in Fig. 2 by curve 1. Parameters α and β are related by equation $\alpha\gamma_1 = \gamma\beta/\sigma_g$. The dependence of $\alpha\gamma_1$ on β is presented in Fig. 2 by curve 2. With increase in β (i.e., in mass m) the force F_- increases while σ_g (and, hence, I_g and F_+) decreases. When the critical loading $\alpha = \alpha_c = 1$ is reached, the buoyant force becomes equal to the weight of pollutant (which corresponds to $\beta = \beta_c$ shown in Fig. 2 for $\gamma_1 = 1$); a further increase in β leads to the buoyancy of the cloud becoming negative.

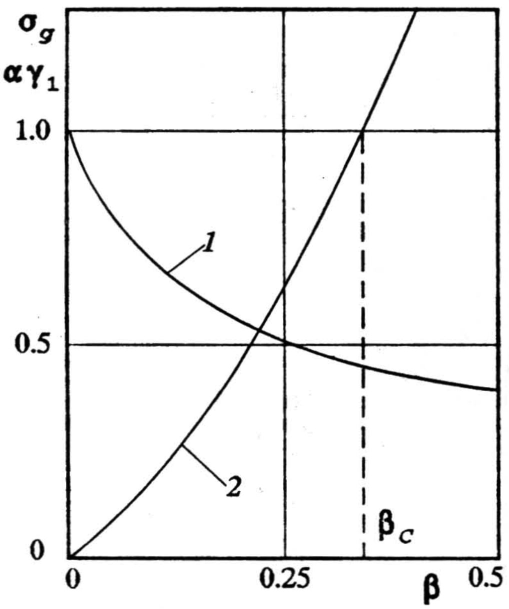


Fig. 2. Fraction of heat stored in gas and ratio of weight of pollutant to total gas buoyancy

Consider first the case $\gamma_1 = 1$ (this value is typical for many kinds of pollutants - dust, sand etc.). The "active" pollutant being considered here can affect the gas motion in two ways. On one hand, the particles make the cloud heavier, on the other hand in presence of disperse pollutant the average heat capacity of the medium increases which gives rise to slower cooling of the gas and favors the ascent of the cloud. Counteraction of these mechanisms governs the dynamics of a dusty thermal. When the loading is less then $\alpha \approx 40\%$, they compensate each other and the self-similar coordinate ξ_t of a dusty thermal is described by (8) where I_0 is to be replaced by I_g. The internal structure and evolution of such a dusty thermal are essentially the same as in case of a gaseous thermal. It doesn't mean, of course, that the pollutant behaves just like a "passive" impurity: in presence of particulate impurity the heat energy of the gas I_g is less than the total heat energy I_0 and the dusty thermal always rises slower than the gaseous cloud provided that the burst energy is the same in two cases. A more heavily loaded thermal is slowed immensely by the pollutant, the influence of disperse phase is most significant at the initial stage. The heavy central "core" brings about the weakening or even the suppression of a convective motion in a near-axis region, whereas at the periphery the concentration is small and a toroidal vortex develops here.

To describe the vertical distribution of pollutant density in the atmosphere after cloud stabilization, introduce the following rescaled variables and parameters:

$$\eta = (z - H_T)/L_S, \quad \kappa = (H - H_T)/L_S, \quad L_S = (I_g/k_1)^{1/4}$$

$$\phi(\eta) = 2\pi L_S m^{-1}\int_0^{\infty} \rho_2 r\,dr, \quad q = \int_{\kappa}^{\infty} \phi(\eta)\,d\eta$$

where L_S correct to constant is equal to the typical stabilization height of the thermal. The definition of L_S basing on I_g allows us to consider both gaseous and particulate clouds.

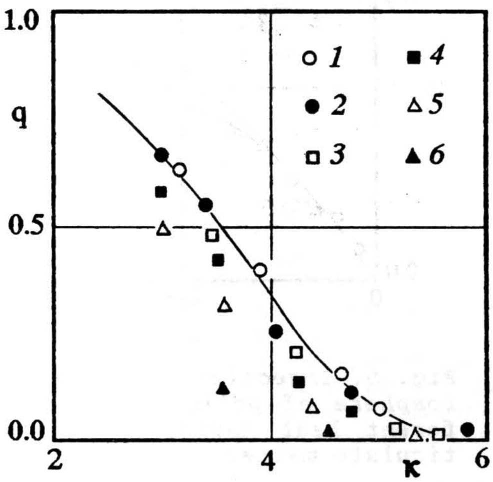
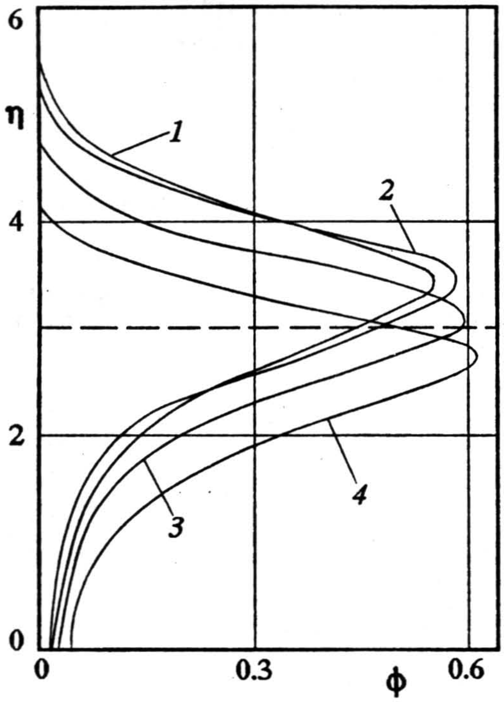


Fig. 3. Fraction of pollutant injected into the stratosphere by a rising thermal

In Fig. 3 the dependence of the fraction of pollutant injected into the stratosphere on κ is presented (note that κ describes the initial position of the thermal relative to the tropopause). All data in Fig. 3 were obtained for I_0 = 0.68 (1 Mt yield burst thermal), H = 1.56, H_T = 9 - 16, γ_1 = 1. The solid line corresponds to the pure gaseous thermal with passive pollutant (which may be regarded as a gaseous pollutant, e.g., NO_x gas). The points 1 - 6 correspond to loadings α = 0.07, 0.2, 0.5, 0.56, 0.7, 0.95. When $\alpha \le \alpha_* \approx 40\%$ the thermal rises just as a gaseous one with energy $I_g < I_0$. That is why the injection of active impurity into the stratosphere can be described by dependence q(k) for "passive" impurity - points 1, 2 lie on the solid curve. When $\alpha > \alpha_*$ the impurity strongly affects the ascent and the fraction of injected pollutant decreases (points 3 - 6).

In Fig. 4 the vertical distribution of impurity in the atmosphere for different loadings $\phi(\eta)$ is presented in case κ = 3. Note that κ depends on I_g which, in turn, depends on loading α , consequently, for fixed κ different α correspond to different altitudes of tropopause H_T. Curves 1 - 4 are plotted for α = 0, 0.2, 0.7 and 0.85, the dashed line denotes the tropopause. It can be seen that the distributions for passive (curve 1) and active impurities differ only slightly when the loading is low (curve 2), whereas for high loadings (curves 3, 4) the maximum of function $\phi(\eta)$ is attained at lower altitudes which gives rise to smaller injection of pollutant into the stratosphere. Finally, in Fig. 5 the dependence of the dimensionless total mass of the pollutant $\mu = \mu_s q$ injected above the tropopause on particle loading level $\mu = m/2\pi I_0$ (or "specific" loading per unit of total heat energy) is presented for different ratios of specific heats γ_1 = 0.25, 1.0 and 2.0 (curves 1 - 3).

It turns out that an increase in the loading of the thermal leads to an increase in injection of impurity only up to a certain limit. A further increase in μ slows down the ascent which results in decrease in μ_s . The maximum injection depends on γ_1 : the smaller is the fraction of initial heat energy stored in particulate phase, the greater is the amount of impurity that can enter the stratosphere.



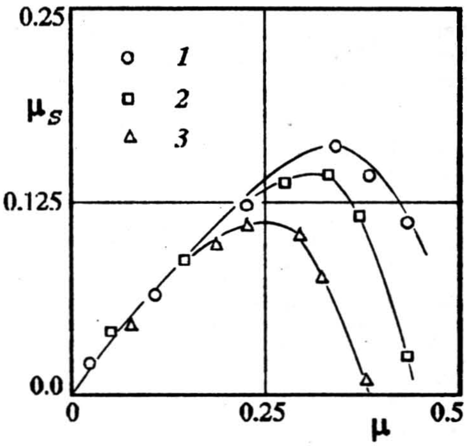


Fig. 4. *Vertical distribution of pollutant formed in atmosphere after the rise of the thermal*

Fig. 5. *Injection into the stratosphere of pollutants for different heat capacities of particulate matter.*

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