# TWO-COMPONENT RADIATION-GASDYNAMIC MODEL OF A TURBULENT FIREBALL

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A two-dimensional computational model of the dynamics of a radiating turbulent fireball that can form in accident-induced explosion of a rocket at the launching position or in flight is presented. The model is based on the system of Navier–Stokes equations, two-component diffusion of explosion products (water vapor) in the ambient air, and a multigroup system of equations of thermal radiation transfer. The possibility of employing three models of turbulent mixing – the Prandtl model, the Penner–Haselman–Edwards model, and the Launder–Spalding model – is investigated.

Introduction. In developing systems for emergency rescue of astronauts or useful cargo in an accidentinduced explosion of a rocket, information on the main damaging factors of this explosion and the distance from the site of the accident at which the action of these factors is safe, must be available. The presence of this knowledge enables developers of emergency rescue systems to solve the problem of selecting the time of separation of the rescued spacecraft (RS) from the rocket: the separation command must be delivered after the inevitability of the accident becomes clear from a set of telemetric parameters but a few seconds before the explosion of the rocket.

It was assumed earlier that this time delay must be determined by the level of a shock-wave load on an RS when a shock wave generated by explosion reaches it. However, as rocket engineering developed and the power of launchers increased, it became necessary to allow for one more damaging factor – thermal radiation of a fireball formed at the site of explosion.

In experimental investigations [1], where the consequences of the explosion of different propellants were studied, it was established that in intertank-partition failure or spilling of propellant components onto the launching position only a small fraction of the mass of the propellant components (~1%) is involved in the explosion phenomenon that accompanies similar accidents. Its major portion burns, evaporating and mixing with the ambient medium. This process lasts for ~10–20 sec, and the cloud of the mixture of propellant components and air formed is referred to as the fireball (Fb). Under the action of Archimedes forces the fireball floats up in the atmosphere with a rate of ~20 m/sec. The size of its cross section depends on the total mass of the propellant. For example, for the Ariane-5 rocket (25 tons of liquid hydrogen and 130 tons of liquid oxygen), the size of the Fb attains ~200 m. Taking into account that the combustion product of this propellant is water vapor radiating intensely in the infrared spectrum and its temperature in the Fb is ~2000 K, it becomes evident that the Fb is an impressive source of thermal radiation that can be a serious hazard to RS in the first 10–20 sec after the explosion at significant distances, where, for example, its parachute opens.

The state of the art in work on semiempirical and numerical modeling of processes that accompany the explosion of a rocket at the launching position or in flight is analyzed in [2]. An engineering semiempirical model of the dynamics and radiation of an Fb is presented in [3], while in [4] it is shown that heat transfer by radiation plays a significant role in its dynamics.

However, as computational models of Fb are developed, it becomes clear that the level of their reliability is still very far from the desired one since they fail to allow for processes that strongly affect the calcula-

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tion results. We indicate only two of them: turbulent mixing and burning down of propellant components in their mixing with atmospheric air.

This work seeks to analyze some models of turbulent mixing when they are employed to close the system of equations of the dynamics of radiating oxygen-hydrogen fireballs.

Mathematical Model. Let the rapid motion of the medium and the chemical reactions of the propellant components leading to formation of hot water vapor be completed by the time taken as the initial instant in the two-dimensional calculation of the dynamics of the fireball (see [2] for the details of different scenarios of the phenomenon). Let us assume that the initial components burned down completely and the ambient air is displaced from the combustion region. Then inside the Fb there are only combustion products, while outside it there is undisturbed air.

These assumptions are used as the basis for a two-component Fb model, in accordance with which the medium consists of water vapor and air. Description of the process of evolution of the indicated two-component mixture of gases including its mixing, cooling down of the fireball, its floating up under the action of Archimedes forces, and heat transfer by radiation within the hot region and with the ambient medium will be the main problem of the formulated computational model.

With allowance for the introduced assumptions of the composition of the medium the dynamics of a turbulent fireball in a two-dimensional coordinate system is described by the following system of equations:

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \left( \rho \, \mathbf{V} \right) = 0 \,, \tag{1}$$

$$\frac{\partial \rho u}{\partial t} + \operatorname{div} \left(\rho u \, \mathbf{V}\right) = -\frac{\partial p}{\partial x} + \frac{S_u}{\operatorname{Re}},\tag{2}$$

$$\frac{\partial \rho v}{\partial t} + \operatorname{div} \left( \rho v \, \mathbf{V} \right) = -\frac{\partial p}{\partial r} + \frac{S_v}{\operatorname{Re}} \,, \tag{3}$$

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p \mathbf{V} \operatorname{grad} T = \frac{1}{\operatorname{Re} \operatorname{Pr}} \operatorname{div} \left(\lambda_{eff} \operatorname{grad} T\right) - \left(c_{p,1} - c_{p,2}\right) \frac{\mu_{eff}}{\operatorname{Re}} \left(\operatorname{grad} c_1 \cdot \operatorname{grad} T\right) - Q \frac{u_0}{c_{p,0} \rho_0 L},$$
(4)

$$\rho \frac{\partial c_1}{\partial t} + \rho \mathbf{V} \operatorname{grad} c_1 = \frac{1}{\operatorname{Re}} \operatorname{div} \left( \mu_{\text{eff}} \operatorname{grad} c_1 \right),$$
(5)

$$Q = \sum_{g=1}^{N_g} \kappa_g \left( U_{b,g} - U_g \right) \Delta \omega_g , \qquad (6)$$

$$\operatorname{div}\left(\frac{1}{3\kappa_g}\operatorname{grad} U_g\right) = -\kappa_g \left(U_{\mathrm{b},g} - U_g\right), \quad g = 1, 2, \dots, N_g = 48,$$
(7)

where

$$S_{u} = -\frac{2}{3} \frac{\partial}{\partial x} \left( \mu_{\text{eff}} \operatorname{div} \mathbf{V} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \mu_{\text{eff}} \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right) \right] + 2 \frac{\partial}{\partial x} \left( \mu_{\text{eff}} \frac{\partial u}{\partial x} \right);$$
  

$$S_{v} = -\frac{2}{3} \frac{\partial}{\partial r} \left( \mu_{\text{eff}} \operatorname{div} \mathbf{V} \right) + \frac{\partial}{\partial x} \left[ \mu_{\text{eff}} \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right) \right] + 2 \frac{\partial}{\partial r} \left( \mu_{\text{eff}} \frac{\partial v}{\partial r} \right) + 2 \mu_{\text{eff}} \frac{\partial}{\partial r} \left( \frac{v}{r} \right);$$
  

$$\operatorname{Re} = \rho_{0} u_{0} L / \mu_{0}; \quad \operatorname{Pr} = \mu_{0} c_{p,0} / \lambda_{0}.$$

Within the framework of this model the process of turbulent mixing is allowed for with Boussinesq's hypothesis by introducing the effective turbulent-viscosity factor  $\mu_t$ , which is determined according to one of the turbulence models. The total effective viscosity factor is found by the formula  $\mu_{eff} = \mu + \mu_t$ .

The effective thermal conductivity is calculated in terms of the Prandtl turbulent number  $Pr_{eff} = \mu_{eff}c_p/\lambda_{eff}$ , which is assumed to be equal to unity, and therefore  $\lambda_{eff} = c_p\mu_{eff}$ .

To determine the diffusion fluxes, in this model use is made of Fick's law  $J_i = -\rho D_i$  grad  $c_i$ , i = 1, 2. It is assumed that because of intense turbulent mixing of the gas we can introduce a unified diffusion coefficient  $D_{\text{eff}} = D_1 = D_2$  that is established by the formula  $\rho D_{\text{eff}} = \mu_{\text{eff}}$ , which is a consequence of the Schmidt turbulent number being equal to unity:  $S_{\text{eff}} = \mu_{\text{eff}}/\rho D_{\text{eff}} = 1$ .

The total density of the medium and the specific heat at constant pressure are calculated by the formulas:

$$\rho = \frac{p_0}{\left(\frac{c_1}{M_1} + \frac{c_2}{M_2}\right)\tilde{R}T}, \quad c_p = c_{p,1}c_1 + c_{p,2}c_2.$$

The partial heat capacities of the water vapor and the air are determined from the data of [5].

To make the system of equations dimensionless, use is made of quantities  $\rho_0$ ,  $c_{p,0}$ ,  $\mu_0$ , and  $\lambda_0$ , which correspond to the undisturbed air atmosphere, and of L and  $u_0 = \sqrt{gL}$ . All the variables in Eqs. (1)-(7) are dimensionless except T.

As the initial conditions we prescribe spherically symmetric distributions of the temperatures and concentrations of the water vapor and the air against the background of the atmosphere at rest

$$\varphi(x, r) = \varphi_0 + (\varphi_c - \varphi_0) \exp\left\{-\left[\frac{\sqrt{(x - x_c)^2 + r^2}}{R_0}\right]^4\right\}, \quad \varphi = [T, c_1, c_2].$$

The initial size of the fireball, with accuracy sufficient for the purposes of this problem, is determined from the mass of the combustion products formed (water vapor)

$$R_0 = \sqrt[3]{\left(\frac{3M_{\rm H_2O}}{4\pi\rho_{x_c}}\right)},$$

where  $M_{\rm H_2O}$  is estimated from the total mass of the propellant components.

The conditions of axial symmetry and "mild" boundary conditions for all the functions are used at the boundaries of the calculated region.

The optical model of the two-component medium is computed at each point of the calculated region  $(r_i, x_i)$  by the following formula:

$$(\mathbf{\kappa}_{g})_{i,j} = (x_1)_{i,j} (\mathbf{\kappa}_{g,1})_{i,j} + (x_2)_{i,j} (\mathbf{\kappa}_{g,2})_{i,j}.$$

In the calculations, we employed a 48-group spectral model of moist air in the spectral range of 1000-10,000 cm<sup>-1</sup> obtained with the use of a MONSTER computer system [6] and experimental data [7].

To prescribe turbulent transfer coefficients, in the present work we use three computational models:

1) the algebraic Prandtl model of turbulent transfer of the simplest form

$$\mu_{t} = \rho l^{2} \sqrt{\left(\left(\frac{\partial u}{\partial r}\right)^{2} + \left(\frac{\partial v}{\partial x}\right)^{2}\right)}; \tag{8}$$

since, for the flows under consideration, there is no theory for prescribing the effective mixing length l, it was estimated from comparison with experimental data [1] on the ascent velocity of a turbulent therm in the atmosphere (l = 0.4-0.6);

2) the algebraic Penner-Haselman-Edwards model of turbulent transfer [8] (in what follows the PHE model), in accordance with which

$$\mu_{t} = \frac{1}{2} \rho l^{2} \sqrt{\left(\left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x}\right)^{2} + 2\left[\left(\frac{\partial u}{\partial r}\right)^{2} + \left(\frac{\partial u}{\partial x}\right)^{2} + \left(\frac{v}{r}\right)^{2}\right]\right)}, \qquad (9)$$

$$\left\{\frac{\sqrt{u^{2} + v^{2}}}{\sqrt{B}} + \sqrt{B} \frac{1}{\sqrt{\left(\left(\frac{\partial^{2} v}{\partial r^{2}} + \frac{1}{r} \frac{\partial v}{\partial r}\right)^{2} + \left(\frac{v}{r^{2}}\right)^{2} + \left(\frac{\partial^{2} v}{\partial x^{2}}\right)^{2} + \left(\frac{\partial^{2} u}{\partial r^{2}} + \frac{1}{r} \frac{\partial u}{\partial r}\right)^{2} + \left(\frac{\partial^{2} u}{\partial x^{2}}\right)^{2}\right)}, \qquad (9)$$

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

where K is an empirical constant with a recommended value of 0.125 [8];

3) the  $k-\varepsilon$  model of turbulent mixing [9], in accordance with which the effective turbulent-viscosity factor is determined by the formula

$$\mu_{\rm t} = C_{\mu} \, \rho k^2 / \varepsilon \, ,$$

and, to calculate the functions k and  $\varepsilon$ , use is made of the following systems of equations:

$$\frac{\partial \rho k}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \left( \rho k v - \frac{\mu_{t}}{\sigma_{k}} \frac{\partial k}{\partial r} \right) \right] + \frac{\partial}{\partial x} \left( \rho k u - \frac{\mu_{t}}{\sigma_{k}} \frac{\partial k}{\partial x} \right) = P - \rho \varepsilon , \qquad (10)$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left[ r \left( \rho \varepsilon v - \frac{\mu_{t}}{\sigma_{\varepsilon}} \frac{\partial \varepsilon}{\partial r} \right) \right] + \frac{\partial}{\partial x} \left( \rho \varepsilon u - \frac{\mu_{t}}{\sigma_{\varepsilon}} \frac{\partial \varepsilon}{\partial x} \right) = (C_{1} P - C_{2} \rho \varepsilon) \frac{\varepsilon}{k}, \qquad (11)$$

where

l = K

$$P = \mu_{t} \left\{ 2 \left[ \left( \frac{\partial v}{\partial r} \right)^{2} + \left( \frac{\partial u}{\partial x} \right)^{2} + \left( \frac{v}{r} \right)^{2} + \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial r} \right)^{2} \right\} - \frac{2}{3} \rho k \left( \frac{\partial u}{\partial x} + \frac{1}{r} \frac{\partial r v}{\partial r} \right) - \frac{\lambda_{t}}{\rho^{2}} \left( \frac{\partial \rho}{\partial r} \frac{\partial p}{\partial r} + \frac{\partial \rho}{\partial x} \frac{\partial p}{\partial x} \right);$$
  
$$C_{\mu} = 0.09 \; ; \quad C_{1} = 1.44 \; ; \quad C_{2} = 1.92 \; ; \quad \sigma_{k} = 1.0 \; ; \quad \sigma_{\epsilon} = 1.3 \; ; \quad \lambda_{t} = c_{p} \; \mu_{t} \; .$$

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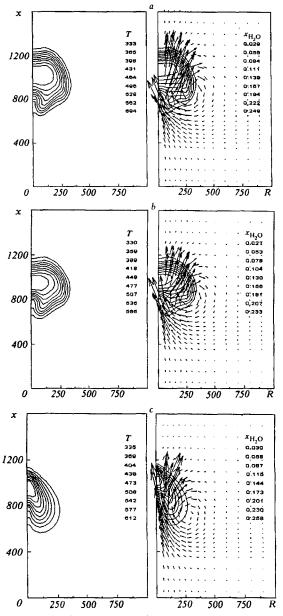


Fig. 1. Thermogasdynamic structure of a two-component fireball within 19 sec after explosion. On the left: the isotherms; the figures on the field of the plot are the temperature in Kelvin; the external isotherm corresponds to the lowest temperature. On the right: the isolines of the concentrations of water vapor and the vector velocity field; the figures on the field of the plot are the relative bulk concentration of water vapor; the external isoline corresponds to the lowest concentration. The arrow length is proportional to the absolute value of the velocity: a) k- $\varepsilon$  model; the highest velocity is 189 m/sec in the positive direction of the x axis and 11 m/sec in the negative direction of the x axis, c) Prandtl model; the highest velocity is 175 m/sec in the positive direction of the x axis and 5 m/sec in the negative direction of the x axis, x, R, m.

The initial conditions for (10) and (11) were selected in accordance with the solution of the equation

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\mu_{t}}{\sigma_{k}}\frac{\partial k}{\partial r}\right) + \frac{\partial}{\partial x}\left(\frac{\mu_{t}}{\sigma_{k}}\frac{\partial k}{\partial x}\right) = P - \rho \frac{k^{3/2}}{L_{t}}, \quad \mu_{t} = C_{\mu} \rho L_{t} k^{1/2}, \quad L_{t} = 0.1R_{0}.$$

In concluding the description of the developed computational model, we will make a number of remarks of general character.

1. The use of the equations of the  $P_1$  approximation of the spherical harmonics method in the problem solved (Eq. (7)) is quite justified, especially, in spectral ranges that correspond to the centers of the absorption bands of water vapor. Where the optical thickness of the entire calculated region is much smaller than unity (the transparence windows of water vapor), one switches automatically to a volumetric-luminescence approximation (this procedure is presented in [10] in detail).

2. In spite of our attempts at analyzing different turbulent-mixing models, we admit that the problem of selecting the most adequate model as applied to the investigated process of Fb dynamics has, unfortunately, not been solved at present. The main reason for this is the absence of experimental data on the dynamics of Fb for the rockets for which the computational models were developed. Furthermore, allowance must be made for the fact that different turbulent-mixing models were created as applied to the boundary-layer flows, so employing them to describe the initial unsteady phase of fireball motion can always be questioned, too. Nonetheless, investigation of different turbulence models is a necessary step toward creating computational procedures intended to establish at least the degree of uncertainty of the results obtained. We notice that similar investigations were performed in a number of works analyzing the dynamics of fireballs generated by a nuclear explosion later in their evolution (see [11] and the analysis of works by other authors performed there).

The system of equations (1)-(7) was solved by the method of unsteady dynamic variables [10].

**Calculation Results.** The calculations were performed as applied to fireballs that can form in the explosion of the Ariane-5 rocket. The initial radius of a homogeneous fireball that consists of water vapor was assumed to be equal to 100 m, while the temperature in it was assumed to be 2970 K. The center of the fireball was located at height  $x_c = 500$  m.

The dynamics of the Fb was tracked up to the 20th sec from the beginning of the process when it ceases to be hazardous as far as thermal radiation is concerned at radial distances of ~500 m.

Figure 1 gives the results of calculating the temperature field in a fireball within 19 sec after the beginning of the process and the isolines of the concentrations of water vapor and the vector velocity field in the fireball for different models of turbulent mixing. The pronounced effect of the type of turbulent-mixing model on the results obtained is obvious. At the same time, taking into account the degree of approximation of the constructed computational model, we see the similarity of the calculated data obtained with the  $k-\varepsilon$  and PHE models. If it is taken into account that the latter model is substantially more economical and contains only one empirical constant (K), it can be recommended for numerical calculations, especially if the possibility exists of estimating the indicated constant from experimental data. We investigated the effect of K. This constant varied within 0.02–0.5. A K variation in the range of 0.1–0.3 was established to have practically no effect on the data obtained. The ascent velocity of the fireball increased strongly as K decreased further and decreased as K increased. In the latter case, we observed an increased rate of cooling of the fireball.

The Prandtl model yields a distorted shape of the fireball as compared to what is obtained according to the  $k-\varepsilon$  and PHE models. This is in agreement with numerous calculated data of other authors. It is well known that this model poorly describes flow in the external region of the boundary layer (in our case, at the periphery of the fireball). At the same time, the highest temperature inside the fireball turns out to be quite similar to the temperature predicted by the other two models. For the same reason, the height of ascent of the fireball also turns out to be very similar.

One more feature of the process of floating up of the fireball is noteworthy. A very intense forced (vortex) downward motion of the gas is observed at a radial distance of ~500 m. The absolute value of this

velocity obtained according to the  $k-\varepsilon$  and PHE models attains ~10 m/sec, which should also be allowed for in developing systems of emergency rescue.

## CONCLUSIONS

1. The computational model of a radiating turbulent fireball that can form in the explosion of a rocket at the launching position or in flight is developed.

2. Three models of turbulent mixing are analyzed; the Penner-Haselman-Edwards model is recommended for use in computational models of the considered class.

3. The dynamics of a fireball that can form in the explosion of an oxygen-hydrogen-propellant rocket (of an Ariane-5 type) is calculated; it is established that by the 19th second after the explosion the fireball cools down to temperatures of  $\sim$  550–600 K and rises to approximately 500 m above the site of the explosion; attention is drawn to the intense vortex motion of the gas in the vicinity of the fireball.

### **NOTATION**

x and r, axial and radial variables; T, temperature; u and v, axial and radial components of velocity V; p, pressure;  $\rho_{x_c}$ , density of combustion products at the explosion height,  $M_{\text{H}_2\text{O}}$ , mass of water vapor;  $\overline{R} = 8.314$ J/(mole·K), universal gas constant;  $\mu_{\text{eff}}$  and  $\lambda_{\text{eff}}$ , effective viscosity factor and thermal conductivity;  $D_{\text{eff}}$ , effective diffusion coefficient;  $\mu$ , dynamic viscosity factor;  $\mu_t$ , turbulent-viscosity factor;  $\kappa$ , U, and  $U_b$ , group absorption coefficient and bulk density of radiant energy of the medium and the ideal black body; L, characteristic space scale; g, free fall acceleration; l, effective mixing length; k, kinetic energy of turbulent motion;  $\varepsilon$ , dissipation rate of turbulent motion;  $R_0$ , initial radius of the fireball;  $\Delta \omega_g$ , spectral range that corresponds to the gth spectral group; K, empirical constant in the PHE model of turbulent mixing;  $u_0$ , scale of the velocity of convective motion. Partial characteristics:  $c_i = \rho_i / \rho$ , mass concentration;  $x_i$ , relative bulk concentration;  $\rho_i$ , density;  $M_1 = 18$  and  $M_2 = 28.8$  kg/kmole, molecular weights of water vapor and air, respectively;  $c_{p,i}$ , specific heat at constant pressure;  $\mathbf{J}_i$ , diffusion flux. Subscripts: i = 1, water vapor; i = 2, air; g, number of the spectral group; 0, parameters in the undisturbed atmosphere; c, location of the center of the fireball at the initial instant; b, ideal black body.

# REFERENCES

- 1. A. B. Willoughy, C. Wilton, and J. A. Mausfield, *Liquid Propellant Explosion Hazards*, Final Report, December 1968, AFRPL-TR-68-98, URS 652-35 (1968).
- 2. S. T. Surzhikov, Teplofiz. Vys. Temp., 35, No. 3, 416-423 (1997).
- 3. S. T. Surzhikov, Teplofiz. Vys. Temp., 35, No. 6, 932-939 (1997).
- 4. S. T. Surzhikov, Dokl. Ross. Akad. Nauk, 359, No. 1, 36-39 (1998).
- 5. L. V. Gurvich, I. V. Veits, V. A. Medvedev, et al., *Thermodynamic Properties of Individual Substances:* Handbook, in four volumes [in Russian], Moscow (1978).
- 6. S. T. Surzhikov, Computational Experiment in Constructing Radiation Models of the Mechanics of Radiating Gas [in Russian], Moscow (1992).
- 7. C. B. Ludwig, Appl. Opt., 10, No. 5, 1057-1073 (1971).
- 8. J. E. Penner, L. S. Haselman, and L. L. Edwards, AIAA Paper, No. 459 (1985).
- 9. V. E. Launder and D. V. Spalding, Comput. Methods Appl. Mech. Eng., 3, 269-289 (1974).
- 10. S. T. Surzhikov. Mat. Modelirov., 7, No. 8, 3-24 (1995).
- 11. A. V. Konyukhov, M. V. Meshcheryakov, and S. V. Utyuzhnikov, *Teplof. Vys. Temp.*, **32**, 236-241 (1999).