SOME THREE-DIMENSIONAL EFFECTS OF HEAT AND MASS TRANSFER IN A FIRE WITHIN A BUILDING

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Results of a numerical investigation of heat and mass transfer at the initial stage of a fire within a building in combustion of a liquid fire load, performed with the use of a three-dimensional mathematical field model, are presented. Formulas approximating the calculation results are proposed for estimation of the maximum time of operation of an opening to release the gas from the building and determination of the size of the zone within which a change in the position of the fire load causes no marked changes in the parameter of heat and mass transfer. Three-dimensional inhomogeneities in the temperature and velocity fields, which have a profound impact on the problem of providing fire safety for buildings, are revealed.

1. Inhomogeneities of the temperature and concentration fields in a fire within a building are of paramount importance in the problems of safe evacuation of people and optimum disposition of fire-alarm detectors [1]. An actual fire represents a complex, incompletely understood, significantly nonstationary, three-dimensional thermogasdynamic process accompanied by a change in the chemical composition of the gas medium. Therefore theoretical study of heat and mass transfer in a fire using three-dimensional models is a topical problem.

2. To investigate the mechanisms of heat and mass transfer in a fire within a building, we use a three-dimensional mathematical field model described in detail in [2, 3]. Here the following main assumptions and simplifications for an actual thermogasdynamic pattern of the process are made:

a) the gas medium in the building is locally, thermodynamically, and chemically equilibrium;

b) the gas medium is a mixture of ideal gases;

c) the velocities and temperatures of the components of the gas mixture are equal at each point of the space;

- d) the chemical reaction of combustion is single-stage and irreversible;
- e) the dissociation and ionization of the medium at high temperatures are disregarded;
- f) turbulent pulsations have no influence on the thermophysical properties of the medium;

g) the mutual influence of turbulence and radiation is ignored.

We solve nonstationary three-dimensional differential equations of the laws of conservation of mass, momentum, and energy for the gas medium of the building (Navier–Stokes equations in the Reynolds form) and for the components of the gas medium and the optical density of the smoke. All the differential equations are reduced to the "standard" form [4] suitable for a numerical solution:

$$\frac{\partial}{\partial \tau} (\rho \Phi) + \operatorname{div} (\rho w \Phi) = \operatorname{div} (\Gamma \operatorname{grad} \Phi) + S, \qquad (1)$$

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Φ	Г	S
1	0	G _m
w _x	$\mu + \mu_t$	$\frac{\partial}{\partial x} \left(\Gamma \frac{\partial w_x}{\partial x} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial w_y}{\partial x} \right) + \frac{\partial}{\partial z} \left(\Gamma \frac{\partial w_z}{\partial x} \right) - \frac{\partial p}{\partial x} - \frac{2}{3} \frac{\partial}{\partial x} \left(\Gamma \operatorname{div} w \right)$
wy	$\mu + \mu_t$	$\frac{\partial}{\partial x} \left(\Gamma \frac{\partial w_x}{\partial y} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial w_y}{\partial x} \right) + \frac{\partial}{\partial z} \left(\Gamma \frac{\partial w_z}{\partial y} \right) - \frac{\partial p}{\partial y} - \frac{2}{3} \frac{\partial}{\partial y} \left(\Gamma \operatorname{div} w \right)$
w _z	$\mu + \mu_t$	$\frac{\partial}{\partial x} \left(\Gamma \frac{\partial w_x}{\partial z} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial w_z}{\partial z} \right) + \frac{\partial}{\partial z} \left(\Gamma \frac{\partial w_z}{\partial z} \right) - \frac{\partial p}{\partial z} - \frac{2}{3} \frac{\partial}{\partial x} \left(\Gamma \operatorname{div} w \right) - \beta g \Delta T$
<i>X</i> _{O2}	$(D_{O_2} + D_{O_2 t})\rho$	$-L_{\mathrm{O}_{2}}$ ψη
X _{CO}	$(D_{\rm CO} + D_{\rm COt})\rho$	L _{CO} ψη
X _{CO₂}	$(D_{\rm CO_2} + D_{\rm O_2 t})\rho$	$L_{ m CO_2}$ ψη
k	μ_t / σ_k	$\nu_{t} \left(\frac{\partial w_{j}}{\partial x_{i}} \left(\frac{\partial w_{i}}{\partial x_{j}} + \frac{\partial w_{j}}{\partial x_{i}} \right) + \frac{g}{\Pr_{t}} \frac{1}{T} \frac{\partial T}{\partial z} \right) - \varepsilon$
ε	μ_t / σ_ϵ	$C_1 \frac{\varepsilon}{k} v_t \left(\frac{\partial w_j}{\partial x_i} \left(\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i} \right) + \frac{g}{\Pr_t} \frac{1}{T} \frac{\partial T}{\partial z} \right) - C_2 \frac{\varepsilon^2}{k}$
W	0	$W_{ m sp}\psi$
i	$\lambda+\lambda_t+\lambda_r$	$\psi \eta Q_{ m w}^{ m low} - Q_{ m r} + \mu \Phi_{ m d}$

TABLE 1. Parameters and Coefficients of Eq. (1)

where Φ is the dependent variable, Γ is the diffusion coefficient for Φ , and *S* is the source term. All the values presented hereafter are time-averaged. The parameters and coefficients of Eq. (1) are presented in Table 1.

We use the $k-\varepsilon$ model of turbulence with the following set of empirical constants [5]: $C_1 = 1.44$, $C_2 = 1.92$, $\sigma_k = 1.0$, $\sigma_{\varepsilon} = 1.3$, and $C_{\mu} = 0.09$. In Eq. (1), the effective gas viscosity is represented in the form $\mu_{\text{eff}} = \mu + \mu_t$, the effective thermal conductivity is represented as $\lambda_{\text{eff}} = \lambda + \lambda_t + \lambda_r$, and the effective diffusion - as $D_{\text{eff}} = D + D_t$.

The viscosity of the gas is determined from the Sutherland formula [5], while the turbulent viscosity is determined from the Kolmogorov formula [5]. The coefficient of turbulent heat conduction is determined from the relation $\lambda_t = c_p \mu_t / Pr_t$, and the coefficient of turbulent diffusion is calculated from the relation $D_t = \mu_t / \rho Pr_d = 1$. We assume that $Pr_t = Pr_d = 1$ [5].

In the calculation of radiative heat transfer in the gas medium we use the approximation of an optically thin layer [6], since below we will perform a numerical investigation of heat and mass transfer at the initial stage of the fire, for which the optical density of the medium outside the flame is low [1]. In this case, $\lambda_r = 0$ in the energy equation, and the formula for calculating the internal sink of heat has the form [6]

$$Q_{\rm r} = 4\pi\gamma\sigma_{\rm r}T^4 \ . \tag{2}$$

In Eq. (2), the integral emissivity of the gas γ is determined from the expression [1]

$$\gamma = 1 - \exp\left(-\theta\delta\right). \tag{3}$$

The coefficient of radiation attenuation is found from the calculated optical density of the smoke [1]:

$$\theta = \lambda^* W \,. \tag{4}$$

The mass rate of gasification of the liquid fire load is equal to [1]

$$\Psi = \Psi_{\rm sp} F_{\rm c} \sqrt{\tau/\tau_{\rm stab}} \,. \tag{5}$$

The rate of release of the optical density of the smoke from the surface of the combustible material is [1]

$$W = W_{\rm sn} \, \psi \,. \tag{6}$$

The region of combustion is specified by volume sources of mass and heat distributed uniformly over the volume of a parallelepiped with a base equal to the area of the fire load and a height $h = 2a_c$.

We set the following boundary conditions for Eq. (1):

a) on the interior surfaces of enclosing structures, the projections of the velocities are equal to zero; for the energy equation, boundary conditions of the third kind are set; for the remaining parameters, it is assumed that $\partial \Phi / \partial n = 0$;

b) in a clear opening, $\partial \Phi / \partial n = 0$ in the region of flow of the gas outward; in the region of flow of the outdoor air inward, the pressure, temperature, and concentration of the components correspond to atmospheric-air parameters.

Equation (1) is solved by the method of control volumes [4] according to an implicit finite-difference scheme on a staggered grid by means of longitudinal-transverse running with the use of an equation for pressure correction in "contractible" form. It is assumed that the distribution of the gas-medium parameters within each control volume corresponds to a scheme with differences in the direction opposite to the flow. The time step is determined from the Courant condition [4], despite the implicit scheme, since it is restricted by the equation for pressure correction.

To perform a reliable calculation of the profiles of the gas-medium parameters and, accordingly, their flows, it is necessary to bunch the grid at the sites where they undergo marked changes (on the walls, in the openings, at the boundaries of the combustion zone, etc.). However, the use of a nonuniform grid also introduces additional errors into the calculations [4]. Because of this, to calculate the heat transfer on the walls, we use experimental values of the coefficients of heat transfer [1]. Here, the main field of the flow is calculated on a uniform grid.

A comparison of the results of calculations performed according to the proposed model on $11 \times 11 \times 11$ and $21 \times 21 \times 21$ finite-difference grids at time steps of $5 \cdot 10^{-4}$ and 10^{-5} sec with the analytical solutions and experimental data has been performed in [2, 3, 7]. Here, the error was no higher than 5 and 20%, respectively. Moreover, the accuracy of the calculations was controlled by fulfillment of the local and integral laws of conservation of mass in the calculational region.

3. The initial data were as follows:

a) the dimensions of the building were $3 \times 3 \times 3$, $6 \times 6 \times 3$, $6 \times 6 \times 6$, and $12 \times 12 \times 12$ m;

b) the upper cut of one opening positioned symmetrically relative to the wall was at the level of the ceiling;

c) the fire load was kerosene of mass M = 50 kg with the following parameters of the process of its gasification [1]: $\psi_{sp} = 0.05$ kg/(sec·m²), $Q_w^{low} = 43.54$ MJ/kg, $W_{sp} = 249$ Np·m²/kg, $L_{CO} = 0.148$, $L_{CO_2} = 2.92$,

 $L_{O_2} = 3.34$, Bu = θd_{eff} , and $d_{eff} = \sqrt{4F_c/\pi}$; the coefficient of absorption and the emissivity of the flame are determined from the Bu number using experimental relations [1];

d) the state parameters of the atmosphere were: temperature, 293 K; pressure, 10^5 Pa; velocity of the wind, 0 m/sec.

In the numerical experiment, the basic parameters of the problem varied within the limits:

a) the value of the openness Π (ratio of the area of the clear opening to the area of the floor) varied from 0.005 to 0.90;

b) the ratio of the height of the clear opening to its width \overline{z} varied from 0.3 to 4.0;

c) the geometric center of the fire load was positioned at the center of the floor at a distance of 0.1L from the clear opening or at a corner of the floor at a distance of 0.1 L from the walls;

d) the ratio of the area of the exposed surface of the fire load, which had the shape of a square, to the area of the floor \overline{F} varied from 0.01 to 0.25;

e) the time of stabilization of combustion of the fire load τ_{stab} varied from 20 to 120 sec.

It was assumed that the initial temperatures of the gas medium within the building, the enclosing structures, and the outdoor air were the same and equal to $T_0 = 293$ K. The temperature of the enclosing structures was assumed to be constant with time. The systems of mechanical ventilation, fire suppression, and heating were switched off.

4. The calculations showed that in the case where the value of the openness is less than 0.01, the opening operates only to release gas from the building throughout the fire, which occurs until the fire load burns out completely or until the oxygen concentration decreases to a value at which the combustion terminates. This result agrees with experimental data [8].

The area of the fire load, the stabilization time of the combustion, the volume occupied by the energy and mass sources (flame), and the presence or absence of convective heat transfer to the enclosing structures or radiative heat transfer in the gas medium outside the region of the flame have a weak influence (a difference of the order of 5%) on the time of operation of the opening to release gas from the building. This conclusion is consistent with results on the influence of the parameters of the problem on the natural gas exchange through a clear opening obtained in [9] according to an integral model for the developed stage of the fire.

Figure 1a shows dependences of the relative time of operation of an opening only to release gas from the building on the value of the openness for different dimensions of the building, on the ratio of the height of the opening to its width, and on the distance of the projection of the center of the opening on the floor to the center of the fire load. Figure 1b shows dependences of this time on the distance of the projection of the center of the opening on the floor to the center of the fire load for different dimensions of the building, different values of the openness, and different values of the ratio of the height of the opening to its width. The relative time was determined as $\tau = \tau_{rel}/\tau^*$, where $\tau^* = \rho_0 V/G^*$ is the characteristic time of the process [1]; $G^* = \rho_0 b H \sqrt{2gH}/2$ is the characteristic flow rate of the gas through the opening.

It is seen from Fig. 1 that the indicated parameters influence substantially the time of operation of the opening to release gas from the building. However, the effect of different parameters is not the same and, for this problem, the principle of multiplicativity of the effects cannot be used to take into account the joint action of several factors. The dependences of the indicated time on these parameters are complex in character and cannot be approximated by simple functions.

For example, in the case where the openness is 0.049, an increase in the ratio of the height of the opening to its width from 1 to 4 causes a decrease in the relative time of operation of the opening to release gas outward and a decrease in this time itself in certain cases of disposition of the fire load.

It is also seen that the influence of the distance from the center of the combustion load to the clear opening on this time is not the same for different values of the openness or for different values of the ratio of the height of the opening to its width. Thus, for $\Pi = 0.049$ ($\overline{z} = 1$), 0.148 (1.33), 0.346 (0.57), and 0.79



Fig. 1. Dependences of the relative time of operation of an opening to release gas outward on the value of the openness (a) and on the distance from the center of the fire load to the plane of the opening (b); a: 1) $\bar{x} = 0.1$; 2) 0.5; 3) 0.9; b: $V = 27 \text{ m}^3$: 1, 2) $\Pi = 0.049$, $\bar{z} = 1.0$ and 4.0; 3, 4) $\Pi = 0.148$, $\bar{z} = 1.33$ and 0.33; 5) $\Pi = 0.346$, $\bar{z} = 0.57$; 6) $\Pi = 0.79$, $\bar{z} = 1.0$, $V = 1728 \text{ m}^3$; 7) $\Pi = 0.346$, $\bar{z} = 0.57$, $V = 108 \text{ m}^3$; 8) $\Pi = 0.173$, $\bar{z} = 0.286$.



Fig. 2. Lines of the same value of \overline{x}_{zone} in the plane $\Pi - \overline{z}$.

(1) the dependence of the relative time of operation of the opening to release gas outward on the above distance is close to linear, while for $\Pi = 0.049$ ($\overline{z} = 4$) and 0.148 (0.33) this dependence is approximately linear up to a distance from the opening to the center of the building and then it remains practically constant.

Thus, for certain parameters of the problem there exists a zone within which a change in the position of the fire load does not cause marked changes in the time of operation of the opening only to release gas from the building or in other parameters of heat and mass transfer. The dimensionless distance along the normal from the plane of the clear opening to the boundary of this zone can be calculated from the results of approximation of numerical calculations with an error no higher than 7% by the following formula:

$$\bar{x}_{\text{zone}} = \Pi^{0.6(\bar{z}-1)} \ \bar{z}^{4.45-22.1\Pi} , \tag{7}$$

where $\overline{x}_{zone} = x_{zone}/L$, x_{zone} is the coordinate of the beginning of this zone along the length of the building, the reference point of which coincides with the plane of the opening. When $\overline{x}_{zone} \ge 1$ the area of this zone is equal to zero.

Figure 2 shows lines of the same \overline{x}_{zone} in the plane $\Pi - \overline{z}$ in accordance with Eq. (7). The picture presented makes it possible to estimate the dimensions of the indicated zone for given values of Π and \overline{z} .



Fig. 3. Temperature fields in the plane perpendicular to the floor: a) the fire load is at the center of the floor; b) the fire load is near the clear opening. z, x, m.



Fig. 4. Dependences of the volume-mean temperature (a) and the mass flow rate (b) on the time from the onset of combustion: 1) analytical solution; 2) integral model ($G_{\rm fl.g}$ and $T_{\rm mean}$); 3) integral model ($G_{\rm ent.a}$); field model: $T_{\rm mean}$, $G_{\rm fl.g}$: 4, 5, 6) the fire load is positioned at the center, at the corner of the floor, and near the clear opening; $G_{\rm ent.a}$: 7, 8, 9) the fire load is positioned at the center, at the corner of the floor, and near the clear opening. $T_{\rm mean}$, K; $G_{\rm fl.g}$, $G_{\rm ent.a}$, kg/sec; τ , sec.

The maximum time of operation of the opening only to release gas outward for given initial data is calculated from the following formula approximating the results of numerical calculations with an error lower than 14%:

$$\overline{\tau}_{\text{max}} = 3.8 \, \frac{0.47 + 0.62\Pi - \Pi^2}{z^{-0.571 - 0.323\Pi}} \,. \tag{8}$$

The time determined from dependence (8) is the minimum time of operation of the opening with a concrete value of the openness to release gas outward, since as the height of the upper cut of the opening decreases on condition that its dimensions remain constant, this time increases and it reaches a maximum value in the case of disposition of the lower cut of the opening at the level of the floor [2, 3].

5. Results of the calculations show that there exist marked inhomogeneities in the temperature, velocity, and concentration fields within the building, which cannot be revealed using integral, zonal, and two-dimensional field models of the thermogasdynamics of a fire.

Figure 3 shows characteristic temperature fields for different positions of the fire load within a building of dimensions $6 \times 6 \times 3$ m for $\Pi = 0.173$, $\overline{F} = 0.01$, $\overline{\tau}_{stab} = 60$ sec, and $\overline{z} = 0.57$. The clear opening is



Fig. 5. Characteristic fields of temperatures (A) and velocities (B) in the plane parallel to the floor and positioned at a distance of 0.15 m from the ceiling in the case where the fire load is positioned at the center (a) and at the corner (b) of the floor. y, x, m.

positioned at the right upper corner of the building. It is seen that in the case where the fire load is positioned in the vicinity of the clear opening (Fig. 3b), only a part of the near-ceiling region is filled with hot gas. Therefore use of zonal models will lead to a qualitatively incorrect result since it is assumed in them that the near-ceiling layer is plane and is entirely filled with a uniformly warmed-up hot gas.

Figure 4 shows results of calculations of the volume-mean temperature of the gas medium within a building, the mass rate of the flow of gas through the opening outward, and the mass rate of the flow of outdoor air inward, performed according to a three-dimensional field model [2, 3], an integral model [9], and an analytical solution [2]. It is seen that the physical pattern of the process at the initial stage of the fire obtained with the integral model is qualitatively and quantitatively incorrect.

The calculated values of the mass rate of the gases flowing outward, obtained according to the model proposed (Fig. 4b, curves 4–6), coincide with the analytical solution with an error no higher than 5% within the time of operation of the opening only to release gas from the building.

Figure 5 shows characteristic temperature and velocity fields in a plane that is parallel to the floor and positioned at a distance of 0.15 m from the ceiling for different located of the fire load. In the figures, the clear opening is locations in the right wall of the building symmetrically relative to its width. It is seen from Fig. 5A that the isotherms corresponding to the near-ceiling region have a fairly complex shape that can be explained by the existence of local regions of accelerated and retarded flows (Fig. 5B). Analogous results have been obtained in [10] for a hermetic building. However, in the case where the fire load is positioned at a large distance from the walls of a building having significantly larger dimensions than the building considered by us, the isotherms in this plane are shaped like concentric circles [10].



Fig. 6. Fields of velocities (A) and temperatures (B) in the plane of the clear opening: a) the fire load is at the center of the floor; b) at the corner. z, y, m.

6. Of great practical importance (for safe evacuation of people) is the position of the surface of equal pressures inside and outside the building, above which hot gases filled with smoke flow outward and below which outdoor air flows in.

Figure 6A shows velocity fields and Fig. 6B shows isotherms in the plane of a clear opening 15 sec after the onset of combustion for different positions of the fire load. It is seen that this surface (Fig. 6A, w = 0 m/sec) is not a plane (as is usually assumed [1]) at the initial stage of the fire, and its shape depends significantly on the relative position of the fire load and the clear opening.

It is also seen from Fig. 6 that in the plane of openings specific two-cell structures arise that gradually merge together as the width of the clear opening decreases. The existence of such inhomogeneities in the parameter fields can introduce significant errors into the measurement of the mass rates of the gases flowing outward and the gases entering the building through the opening. For example, the experimental values of the mass rates presented in [1] were obtained when the corresponding transducers were positioned along the vertical axis of symmetry of the opening, i.e., the inhomogeneities of the gas flow along the width of the building were not taken into account.

CONCLUSIONS

1. When zonal and integral mathematical models of the thermogasdynamics of a fire are used to calculate its initial stage, the results obtained can be qualitatively and quantitatively incorrect.

2. The formulas obtained for calculating the maximum time of operation of the opening only to release gas from the building and for determinating the size of the zone of mutual "insensitivity" of the fire load and the opening can be used to refine the integral model of the thermogasdynamics of a fire at its initial stage.

3. The three-dimensional effects of heat and mass transfer in a fire within a building revealed in the numerical experiment are of prime importance, and they should be taken into account in considering the problems of safe evacuation of people and disposition of fire-alarm detectors.

NOTATION

T, temperature; ρ , density; p, pressure; τ , time; τ_{rel} , time of operation of the opening only to release gas outward; w, velocity; G, mass flow rate of the gas; G_m , internal source of mass; Π , openness; c_p , specific heat at constant pressure; ψ , rate of gasification of the combustible material; \overline{z} , ratio of the height of the clear opening to its width; L, length of the building; x, y, z, coordinates along the length, width, and height of the building, respectively; $\overline{x} = x/L$, dimensionless coordinate; γ , integral emissivity of the gas layer; δ , thickness of the gas layer; λ^* , coefficient for recalculating the optical radiation range to the infrared range; θ , coefficient of attenuation of radiation from a gas medium of thickness δ ; λ , μ , ν , and D, coefficients of molecular heat conduction, kinematic and dynamic viscosity, and diffusion, respectively; Pr and Pr_d, Prandtl number and diffusional Prandtl number; i, enthalpy; g, free-fall acceleration; k, kinetic energy of turbulence; ε , dissipation rate of the kinetic energy of turbulence; β , coefficient of volumetric thermal expansion; Q, internal volume source of energy; Q_w^{low} , lower working heat value; X, mass concentration of the gas; η , completeness of combustion; F_c, area of the exposed surface of the combustible material; F, ratio of the surface area of the fire load to the area of the floor; a_c , length of the fire load; Bu, Bouguer number; M, mass of the fire load; $L_{\rm CO}$ and $L_{\rm CO_2}$, mass of carbon monoxide and carbon dioxide released in combustion of 1 kg of combustible material; L₀, mass of oxygen consumed in combustion of 1 kg of combustible material; W, optical density of the smoke; σ_r , Stefan-Boltzmann constant; *n*, normal to the surface; *H*, half the height of the building; *V*, volume of the building; b, width of the opening; Φ_d , dissipation function; d, diameter; C_1 , C_2 , σ_k , σ_ϵ , and C_{μ} , constants. Subscripts: mean, volume-mean parameters of the gas medium in the building; sp, specific parameters; ent.a, air entering the building; fl.g, gases flowing outward; stab, stabilization of combustion; zone, boundary of the zone of insensitivity of the parameters of heat and mass transfer to the coordinates of the center of the fire load; 0, parameters at the initial instant of time; f.load, geometric center of the fire load; eff, effective values of the parameters; c, combustible material; x, y, and z, projections on the coordinate axes; t, turbulence; r, radiative heat transfer; i and j, projections on coordinate axes differing from one another; d, diffusion; rel, release.

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