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SPECIAL FEATURES OF PROPAGATION OF HYDROGEN IN A BUILDING

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A three-dimensional mathematical model for calculating heat and mass transfer in propagation of hydrogen in a building that allows for gas exchange with the environment through an opening has been proposed. Based on numerical calculations performed by the proposed model, the author revealed certain features of the concentration fields of hydrogen in the case of its inflow at the floor level. It is shown that the dimensions and location of the explosion- and fire-hazardous zones change considerably during the process.

1. The regularities of formation of explosive hydrogen–air mixtures in the case of inflow of hydrogen to the upper part of a large-volume building have been studied rather extensively [1]. The characteristic time of equalization of the concentrations of hydrogen over the entire volume of the building is of the order of several hours. In the case of inflow of hydrogen to the lower part of the building this time is of the order of several minutes, which is asserted in [1, 2] without any experimental data. This is associated with the difficulty of measuring rapidly changing concentrations this gas [3]. Therefore, the study of the regularities of formation of explosion- and fire-hazardous concentrations in the case of inflow of hydrogen to the lower part is an urgent problem.

2. A three-dimensional mathematical model for calculation of heat and mass transfer in propagation of hydrogen in a building with openings has been proposed in the paper. The model allows calculation of the concentration fields of hydrogen with arbitrary boundary and initial conditions. The model also accounts for such flow-disturbing factors as nonisothermicity, compressibility, longitudinal and transverse gradients of pressure, roughness, and injection-suction on the surfaces of protecting structures. It involves solution of nonstationary three-dimensional differential equations of the laws of conservation of mass, momentum, and energy for the gas medium of the building and the law of conservation of mass for the hydrogen. All the differential equations are reduced to a "standard" form [4] convenient for numerical solution:

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

where Φ is a dependent variable (the enthalpy, the projections of the velocity on the coordinate axes, the concentration of the hydrogen, the kinetic energy of turbulence, and the rate of turbulence dissipation); Γ is the diffusion coefficient for Φ; S is the source term. The parameters and coefficients of Eq. (1) are given in Table 1. The coordinate axes, which are parallel to the length, width, and height of the building, are denoted by x, y, and z, respectively. All the quantities presented hereafter are time-averaged.

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

The gas viscosity is determined by the Sutherland formula [5], and the turbulent viscosity by the Kolmogorov formula [5]. The coefficient of turbulent thermal conductivity is found from the relation $\lambda_t = c_p\mu_t/\mathrm{Pr}_t$, and the coefficient of turbulent diffusion of hydrogen is determined from the expression $D_t = \mu_t/\rho\mathrm{Pr}_d$.

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

Φ	Γ	S
1	0	$G_h/\Delta V$
w_x	$\mu+\mu_t$	$-(\partial p/\partial x)$
w_y	$\mu+\mu_t$	$-(\partial p/\partial y)$
w_z	$\mu+\mu_t$	$-(\partial p/\partial z)-\beta g\Delta T$
X_h	$(D+D_t)\rho$	$G_h/\Delta V$
i	$\lambda+\lambda_t$	q_h

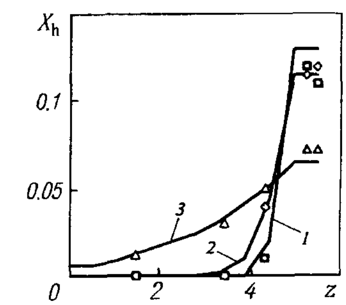

Fig. 1. Distributions of hydrogen concentrations over the height of the building at different instants, calculation by (1): 1) τ = 1200 sec; 2) 2400; 3) 4800; points, experiment [1]. z, m.

For Eq. (1), the following boundary conditions are set:

(a) at the interior surfaces of the protecting structures, the projections of the velocities are zero; for the energy equation, boundary conditions of the third kind are set; for the remaining parameters, $\partial\Phi/\partial n = 0$, where n is the normal to the surface;

(b) at an opening, $\partial\Phi/\partial n = 0$ in a region of gas outflow, while in a region where outdoor air enters the building, the pressure and temperature correspond to the parameters of atmospheric air and the mass concentration of the hydrogen is zero.

Equation (1) is solved by the method of control volumes [6] according to an implicit finite-difference scheme on a staggered grid using longitudinal-transverse running. In this case, an equation for pressure correction in a "contractible" form is used. The distribution of the parameters of the gas medium within each control volume is taken to be different (to correspond to a scheme where these parameters are different in the direction counter to the gas flow, a power law, and an exponential solution).

To reliably calculate the profiles of the parameters of the gas medium and, accordingly, of the gas flows, it is necessary to bunch the grid at the sites where the parameters change significantly (on the walls, at the openings, at the boundaries of the combustion zone, and so on). However, the use of a nonuniform grid introduces additional computational errors [4]. Therefore, we use the integral method of calculation of the boundary layer [6] with a number of refinements [7] to calculate friction and heat transfer on the walls. Here, the main flow field is calculated on a uniform grid.

3. We performed numerical calculations for a building with dimensions $B \times L \times H = 3 \times 3 \times 3$ m. One opening 2 m in width and 1.2 m in height is positioned symmetrically along the width of a wall. The upper cut of the opening is at the level of the ceiling. The parameters of the atmosphere are as follows: temperature, 293 K; pressure, 10^5 Pa; wind velocity, 0 m/sec. The gas medium in the building is considered to be a mixture of ideal gases (air and hydrogen). It is assumed that the temperatures of the gas medium in the building, the protecting structures, the hydrogen entering the building, and the outdoor air are the same. At the initial instant the mass concentration of hydrogen in the building is taken to be zero.

The inflow of hydrogen into the building is simulated by specifying a source of the mass of hydrogen at the center of the floor with a mass flow rate G_h = 0.004 kg/sec constant in time at a height of 0.3 m from

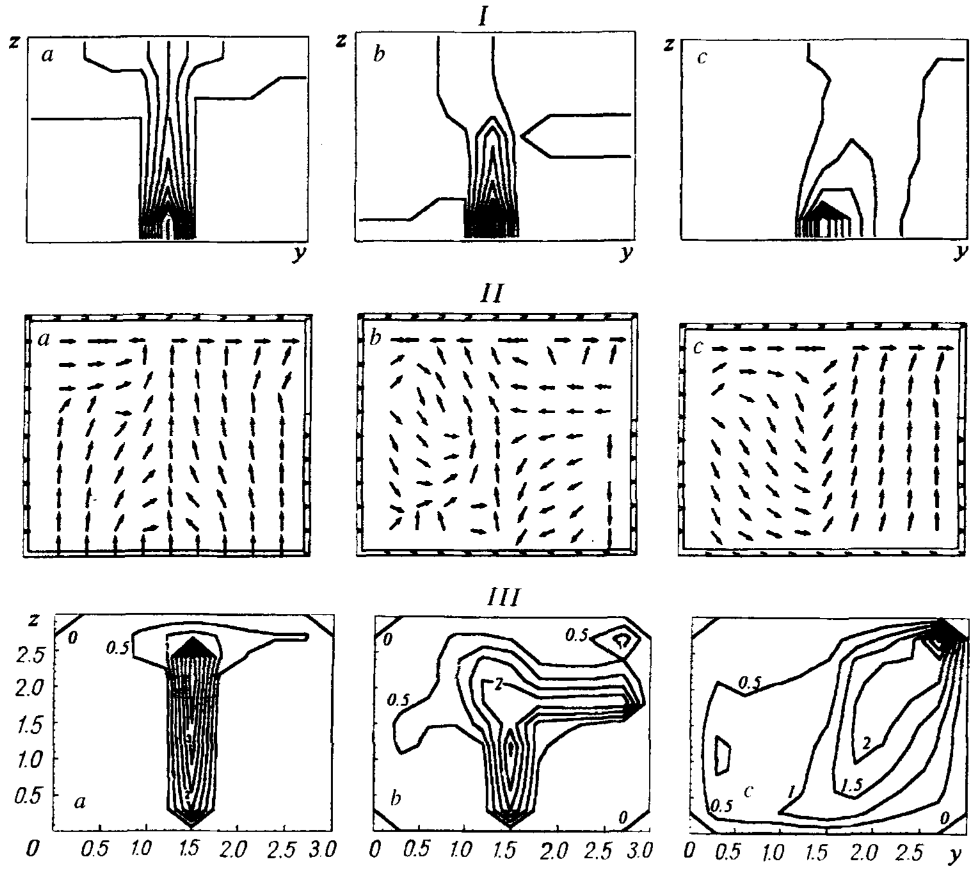

Fig. 2. Concentration field of hydrogen (*I*), scheme of the flow (*II*), and velocity field (*III*) at different instants: a) τ = 10 sec; b) 50; c) 120.

the floor level within one control volume (ΔV = 0.027 m^3). The initial data are taken from [8] for the case of hydrogen outflows from a hydride accumulator under the thermal effect of a fire.

We controlled the accuracy of the calculations by fulfillment of the local equation of conservation of mass in the calculation region. The results of calculations performed using different approximations of the distributions of the parameters of the gas medium in the control volume, different numbers of nodal points of the uniform finite-difference grid (11 × 11 × 11 and 21 × 21 × 21), and different time steps (from 10^{-5} to $5 \cdot 10^{-4}$ sec) coincide with an error of no more than 8%.

4. Figure 1 presents results of comparing calculated and experimental [1] distributions of local volume concentrations of hydrogen over the height of the building in the case of inflow of hydrogen to its upper part. The coincidence of the calculation by the suggested technique and the experimental data is satisfactory for an engineering method of calculation.

Figure 2 *I* presents lines of the same mass concentration of hydrogen, and Fig. 2 *II* and *III* shows schemes of flow and lines of equal velocities in the plane that passes through the center of the floor and is perpendicular to the planes of the floor and the wall with the opening at different times after the start of the inflow. Dependences of the local mass concentrations of hydrogen at several characteristic points of the building on the time from the start of hydrogen inflow are presented in Fig. 3.

It is clear from Figs. 2 and 3 that the physical pattern of flow inside the building at different instants is significantly different. For example, the mass concentration of hydrogen at the ceiling above the source of hydrogen (Fig. 3, curve 3) does not change for a certain period of time (of the order of 10 sec). This period of the inflow can be called the regime of undeveloped convection, since here substantial convective processes do not completely cover all zones of the building. It is seen from Fig. 2a that during this time a vertical con-

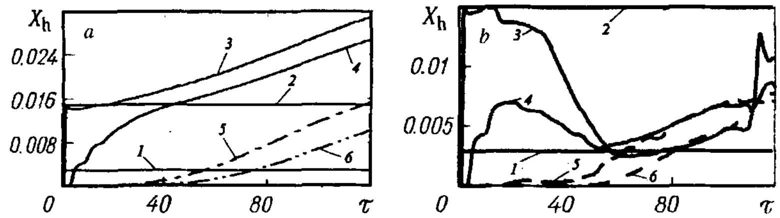

Fig. 3. Mass concentrations of hydrogen vs. time: a) airtight building; b) building with an opening; 1, 2) lower limit of combustion and detonation; 3, 4) center and corner of the ceiling; 5, 6) wall at the level of half the height of the building and the floor. τ, sec.

vective column that is similar to the case of fire is formed above the source of hydrogen [9]. The fields of the gas-medium parameters are symmetric relative to the vertical axis of the column with slight deviations near the opening. The local concentrations of hydrogen in different parts of the building differ significantly (Fig. 3).

Then, in the mode of developed convection (after 10 sec) relative equalization of the concentrations of hydrogen over the volume of the building within limits of the order of 0.3 wt.% (Fig. 3) occurs in about 80 sec. During this time the fields of the parameters of the gas medium are substantially nonsymmetric relative to the convective column, whose axis of symmetry deviates greatly from the vertical direction (Fig. 2b and c). 100 sec after the start of the inflow, the local concentrations of hydrogen at the ceiling above the source increase sharply (Fig. 3, curve 3). This is caused by a change in the flow pattern of the gas medium, which is seen from Fig. 2 *II*, b and c. Here, the scheme of gas exchange through the opening (Fig. 2 *II*, b) 120 sec after the start of the inflow is close to the corresponding scheme 10 sec after (Fig. 2 *II*, a). Thus, the physical pattern of the flow changes periodically. This conclusion is confirmed by calculations with variation of the area of the opening. Calculations further over time were not conducted due to the large consumption of personal-computer time.

Under the given conditions of the problem a region with a concentration of hydrogen higher than the lower limit of detonation lies in the region of the convective column above the source of hydrogen, and it greatly changes its dimensions during the inflow. For example, in 2 sec it reaches the front point of the convective column on the ceiling (Fig. 2 *I*, a). 50 and 120 sec after the start of the process, the height of this region is equal to half the height of the building (Fig. 2 *I*, b and c).

Up to a time of about 60 sec, the region with a concentration of hydrogen higher than the lower limit of combustion consists of the convective column and a near-ceiling layer with its lower boundary lying above half the height of the building (Fig. 3). After 60 sec this lower boundary passes into the lower half of the building, and in 80 sec it reaches the level of the floor (Fig. 3), i.e., it covers the entire building except for a small region near the lower half of the opening.

In an airtight building, the region with a concentration of hydrogen higher than the lower limit of detonation, in contrast to a building with an opening, increases continuously with time, and in 150 sec it occupies the entire building (Fig. 3a). The region with a concentration of hydrogen higher than the lower limit of combustion also increases continuously, and in 75 sec it occupies the entire building.

Up to a time of 30 sec from the start of the process, the physical pattern of hydrogen inflow to the lower part of a building with an opening is similar to the pattern appearing in the initial stage of fire (in combustion of a fire load a source of heat and mass is specified instead of a source of hydrogen mass) [9]. After this the analogy is violated, i.e., there is no symmetric suction into the lower part of the convective column (Fig. 2 *II*, b and c). This can be explained as follows. The density of the gas medium above a source of combustion is determined by processes of convection and radiative heat transfer from the flame. In the case of a hydrogen source, the density above it is determined just by convection. Therefore, with comparable initial and boundary conditions of the problem, the density of the gas medium above the source of hydrogen is substantially lower, and hence the pressure fields in the gas medium of the building differ significantly.

CONCLUSIONS

1. Using the developed three-dimensional mathematical model of heat and mass transfer in the case of inflow of hydrogen to a building, we reveal local regions within the building where explosion- and fire-hazardous concentrations of hydrogen are formed.

2. It is shown that the dimensions and location of explosion- and fire-hazardous zones change substantially during the process.

3. We found an analogy of the physical pattern of the flow of the gas medium in a building in the initial stages of propagation of hydrogen and fire.

NOTATION

ρ, density; c_p, specific heat at constant pressure; τ, time; p, pressure; w, velocity; λ, μ, and D, coefficients of molecular thermal conductivity, viscosity, and diffusion, respectively; G, mass flow rate of the gas; B, L, and H, width, length, and height of the building; $\mathrm{Pr_d}$ and $\mathrm{Pr_t}$, diffusion and turbulent Prandtl numbers; i, enthalpy; g, free-fall acceleration; β, coefficient of volumetric thermal expansion; q, volumetric source of energy; X, mass concentration of the gas; σ, constant. Subscripts: h, hydrogen; t, turbulence.

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