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CALCULATION OF THE DIMENSIONS AND DYNAMICS OF THE FORMATION OF LOCAL EXPLOSION-HAZARDOUS ZONES IN PROPAGATION AND COMBUSTION OF HYDROGEN WITHIN A BUILDING

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On the basis of numerical calculations by a three-dimensional mathematical model, the author revealed some special features of heat and mass transfer within a building in the inflow of hydrogen at the floor level and subsequent detonation combustion of a local hydrogen–air mixture upon its ignition on the ceiling surface. By generalizing calculation results, the author obtained formulas for determining the height of a local explosion-hazardous zone which is formed above the source of hydrogen inflow. It is shown that in detonation combustion, local explosion- and fire-hazardous zones near the source of ignition can be destroyed and shifted to the lower and upper parts of the building toward the wall which is opposite to the opening.

1. To substantiate scientifically the evaluation of fire and explosion hazard within buildings where a hydrogen power plant is installed or work with hydrogen is done, one must know the laws of formation of local explosion-hazardous zones and combustion of a hydrogen–air mixture within them. The propagation and combustion of hydrogen within a building are a substantially nonstationary and three-dimensional heat- and mass-transfer process. However, results of theoretical investigations of this process with the use of three-dimensional mathematical models have not been sufficiently reflected in the literature [1] and cannot serve as a basis for the development and revision of the norms of fire and explosion safety in using hydrogen.

2. A numerical experiment is conducted with the use of a three-dimensional mathematical model for calculating heat and mass transfer within a building with openings in propagation and combustion of hydrogen, which is described in [2-5] in detail. Simultaneously, the author solves nonstationary three-dimensional differential equations of the laws of conservation of mass, momentum, and energy for a gas medium within a building (the Navier–Stokes equations in Reynolds form) and for its components. Comparison of the results of the calculation by the suggested model with experimental data on heat and mass transfer in fire and on concentration fields of hydrogen [2-5] showed an accuracy which is satisfactory for an engineering method of calculation.

The system of differential equations is solved by the method of control volumes [6] according to an implicit finite-difference scheme on a staggered grid by way of longitudinal-transverse running. In this case, the equation for a pressure correction in "contractible" form is used. The distribution of the parameters of the gas medium within each control volume is taken to be corresponding to an exponential solution. We use the integral method of calculation of the boundary layer [7] with a number of refinements [8] to calculate the friction and heat transfer on the walls. The basic field of flow is calculated on a uniform grid.

We controlled the accuracy of the calculations through the fulfillment of the local and integral equations of conservation of mass in the calculation region. The results of the calculations performed with the use of different approximations of the distributions of the gas-medium parameters within the control volume, a different number of nodal points of the uniform finite-difference grid ($11 \times 11 \times 11$ and $21 \times 21 \times 21$), and different time steps (from 10^{-6} to $5 \cdot 10^{-4}$ sec) coincide with an error of no more than 8%.

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3. The effect of the basic parameters of the problem on the height of the explosion-hazardous zone formed above the source of hydrogen inflow has been studied numerically in the mode of nondeveloped convection [2]. The following initial data are taken:

• the dimensions of the building are 3 × 3 × 3 and 6 × 6 × 6 m;

• one opening has an openness (the ratio of the area of the opening to the area of the floor) equal to 0.346; the upper cut of the opening is set at the level of the ceiling; the vertical axis of the opening is positioned symmetrically along the wall of the building; the ratio of the height of the opening to its width is 0.57;

• the inflow of hydrogen into the building is simulated by assigning the source of the hydrogen mass at the center of the floor with the time-constant specific mass flow rate varying within the range j_h = 0.01–0.1 kg/(sec·m^2) at a height of 0.3 m (or 0.6 m);

• the effective diameter of the opening through which hydrogen enters varies within the limits d_{eff} = 0.2–0.7 m;

• the systems of mechanical ventilation and heating are switched off.

The initial data correspond to laminar and transient modes of an isothermal flow of hydrogen at the outlet section of the opening.

The initial conditions are taken as follows:

• the temperatures of the gas medium in the building and protecting structures are 293 K;

• the pressure in the gas medium of the building at the floor level is 10^5 Pa;

• the mass concentrations of oxygen and nitrogen are X_{O_2} = 0.23 and X_{N_2} = 0.77, respectively (mass concentrations of other gases are zero).

The boundary conditions are:

• the parameters of the state of the atmosphere are: temperature 293 K; pressure at the level of the floor 10^5 Pa; wind velocity 0 m/sec;

• in the opening $\partial\Phi/\partial n = 0$ in the region of gas outflow, where Φ is the dependent variable (enthalpy of the mixture, projections of the velocity on the coordinate axes, concentrations of the gas-mixture components, kinetic energy of turbulence and rate of its dissipation) [2-5], n is the coordinate along the normal to the plane of the opening; in the region where the outdoor air enters the building, the pressure, temperature, and concentration of the components correspond to atmospheric-air parameters;

• at the interior surfaces of the protecting structures, the projections of the velocities are zero (the condition of sticking); for the remaining variables, $\partial\Phi/\partial n = 0$.

4. The results of calculating the dependence of the maximum height of the explosion-hazardous zone above the source of the inflow of hydrogen on the basic parameters of the problem are approximated, with an error of no more than 3%, by the following relation:

$$\overline{H}_{\text{e-h.z}} = (-0.55 + 63.78\,\overline{j}_{\text{h}} - 2227\,\overline{j}_{\text{h}}^{\,2} + 58080\,\overline{j}_{\text{h}}^{\,3})\left(\frac{H}{5.7}\right)^{-1.5}, \tag{1}$$

where $\overline{H}_{\text{e-h.z}} = H_{\text{e-h.z}}/d_{\text{eff}}$ is the dimensionless height of the explosion-hazardous zone, $H_{\text{e-h.z}}$ is the height of this zone, H is the height of the building, $\overline{j}_{\text{h}} = j_{\text{h}}/j_{\text{sc}}$ is the relative specific mass flow rate of the entering hydrogen, and j_{sc} = 1 kg/(sec·m^2) is the scale of the specific flow rate.

When dimensionless parameters, similar to those presented in [9], are used in the analysis of heat and mass transfer in a fire within the building, the formula for determining the height of the explosion-hazardous zone with an error of no more than 22% has the form

$$\overline{H}_{\text{e-h.z1}} = (1000\,\overline{j}_{\text{h1}})^{31.62\sqrt{\overline{j}_{\text{h1}}}}, \tag{2}$$

where $\overline{H}_{\text{e-h.z1}} = H_{\text{e-h.z}}/(\sqrt{F}/H)$ is the dimensionless height of the explosion-hazardous zone, F is the area of the opening through which the hydrogen enters, $\overline{j}_{\text{h1}} = j_{\text{h}}/j_{\text{sc1}}$ is the relative specific mass flow rate of the en-

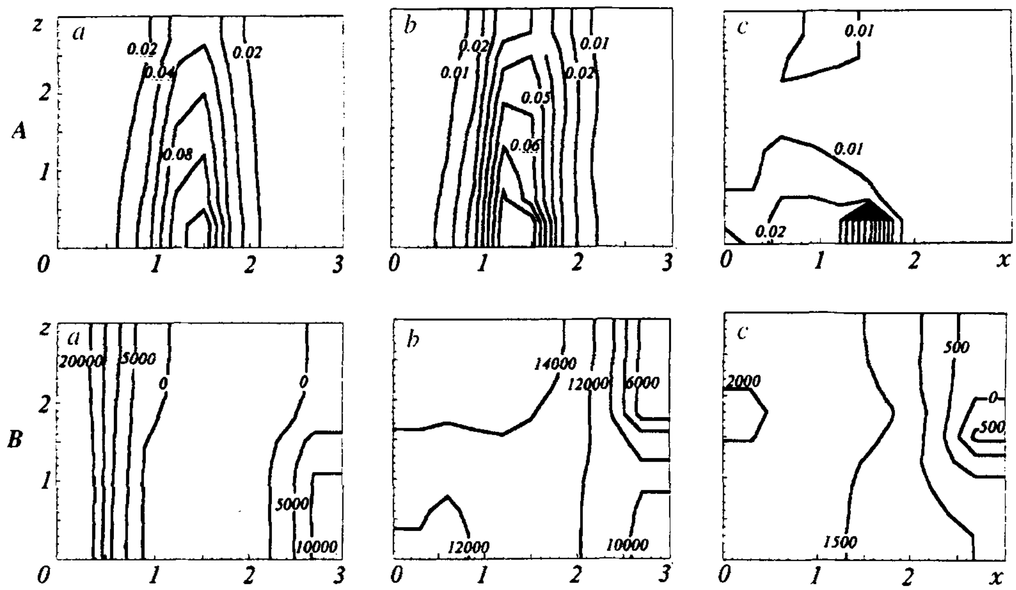

Fig. 1. Fields of mass concentrations of hydrogen (A) and excess pressure (B) at different instants of time from the onset of combustion: a) τ = 0.0005 sec; b) 0.01; c) 0.1. z, x, m.

tering hydrogen, $j_{sc1} = \rho\sqrt{gH}$ is the scale of the specific mass flow rate, $\rho = 1.19$ kg/m^3 is the density of the outdoor air, and g is the free-fall acceleration.

The calculations by the relations for a free turbulent or laminar convective jet will give an underestimated value of the maximum height of the explosion-hazardous zone compared to the values that are obtained by Eqs. (1) and (2), since the maximum height of this zone will be in the mode of nondeveloped convection in the initial stage of the process [2] during which the jet is in the process of formation.

An analysis of the calculation results showed that the openness, the coordinates of the edges of the openings and their number, and the coordinate of the center of the source of the inflow of hydrogen weakly (less than 5%) affect the maximum height of the explosion-hazardous zone.

5. The special features of heat and mass transfer in combustion of a local inhomogeneous hydrogen–air mixture within the building with the opening with account for the dynamics of its formation are studied numerically. At the level of 0.3 m from the floor within one control volume (0.3 × 0.3 × 0.3 m) in the building with dimensions 3 × 3 × 3 m there is a source of hydrogen inflow with a rate of G_h = 0.04 kg/sec. The remaining initial data and the initial and boundary conditions coincide with those presented earlier.

When, in the region of the convective column, which is formed above the source of hydrogen and touches the surface of the ceiling, the concentration of the hydrogen exceeds the lower concentration limit of detonation, the mixture is ignited over the entire area of contact of the mixture with the ceiling surface. The flame front propagates over the mixture at a velocity of 2.7 m/sec [10]. The combustion stops when the concentration of the hydrogen in the combustion region becomes smaller than the lower limit of concentration.

The calculations show that with the appearance of the convective column above the source of hydrogen, the concentration of the hydrogen on its leading front immediately exceeds the lower concentration limit of detonation (the mode of nondeveloped convection [2]) and ignition occurs at the instant when the front of the column touches the surface of the ceiling.

Figure 1A shows the fields of mass concentrations of hydrogen at different instants of time from the onset of combustion in the plane which is perpendicular to the floor and the opening (at the right upper corner of the figure) and passes through the center of the building. Figure 1B presents the field of excess pressure in the same plane at the corresponding instants of time, and Fig. 2 shows the schemes of flow.

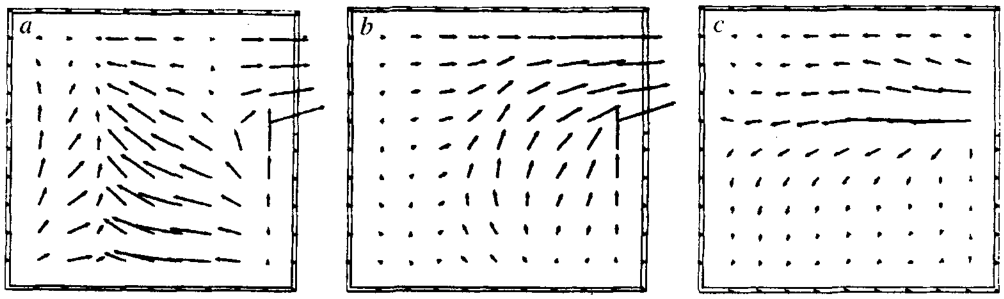

Fig. 2. Schemes of flow at different instants of time from the onset of combustion: a-c) same as in Fig. 1.

It is seen from Figs. 1 and 2 that the gasdynamic pattern of the process has a complex character. After 0.0005 sec from the onset of combustion, the entire hydrogen is in the region of the convective column (Fig. 1A, a). Here virtually lies a low-pressure region. After 0.005 sec from the onset of combustion, the region with hydrogen spreads in a direction that is nearly perpendicular to the axis of the column (Fig. 1A, B).

After about 0.005 sec, the convective column begins to collapse. Under the action of the jet of outdoor air which arises as a result of the difference of pressures inside and outside of the building (Fig. 2c), the local zones with an explosion- and fire-hazardous concentration of hydrogen shift to the source of inflow and move away from the opening, with the region with the highest concentration of hydrogen being near the floor (Fig. 1A, c). Therefore, in the presence of other sources of ignition on the walls or at the floor level, new ignition of the mixture is possible. In this case, the concentration of the hydrogen on the existing combustion front becomes smaller than the lower detonation limit of combustion and the character of the latter becomes "quasistationary."

CONCLUSIONS

1. The maximum height of the explosion-hazardous zone formed above the source of the inflow of hydrogen at the floor level greatly depends on the specific mass flow rate of the hydrogen and the height of the building. The openness, the coordinates of the edges of the openings and their number, and the coordinates of the center of the source of hydrogen inflow weakly affect this height.

2. Under the conditions of continuous inflow of hydrogen, in the detonation combustion of local hydrogen–air mixtures, which are nonuniform with respect to concentration, the destruction of local explosion- and fire-hazardous zones under the ceiling, the shift of these zones to the lower part of the building toward the wall opposite to the wall with the opening, and a change of the detonation character of combustion to "quasistationary" are possible.

NOTATION

τ, time; G, mass flow rate of the gas; j, specific mass flow rate of the gas; X, mass concentration of the gas; x and z, coordinate axes along the length and height of the building, respectively; d, diameter of the opening. Subscripts: h, hydrogen; e-h.z, explosion-hazardous zone; sc, scale of the corresponding parameter; eff, effective value.

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