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HEAT AND MASS EXCHANGE IN COMBUSTION OF A LIQUID COMBUSTIBLE MATERIAL IN A ROOM WITH AN OPEN APERTURE

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An integrated mathematical model of heat and mass exchange for fire in a room that has open apertures is suggested. The results of numerical investigation are presented for the effect of the fundamental parameters of the problem on the mean volumetric parameters of the gaseous atmosphere of the room, the temperatures of the enclosing structures, and on the parameters of the natural gas exchange with the environment through an open aperture in the case of combustion of a liquid combustible material.

1. Simulation of heat and mass exchange in a gaseous atmosphere in a room on fire that has open apertures is an extremely complex problem that has not been completely solved [1]. Turbulent convective and radiative heat and mass exchange at a site of combustion with chemical reactions, heat exchange between the hot gases and enclosing structures (ES) of the room, and so on are complicated by heat and mass exchange with the environment through apertures and due to the operation of systems of forced plenum and exhaust ventilation and fire-fighting.

The majority of published experimental data on heat and mass exchange in a room on fire that has open apertures lack complete information on the experiment conditions. Works [1, 2] are an exception, but they cite the results on combustion of a solid combustible load (CL), namely wood. There are virtually no such experimental data in the literature for combustion of a liquid CL.

The speed of the spread of flame over a surface, the specific heat of combustion, and the rate of gasification of a liquid CL are substantially higher than for a solid CL [1]. As a result, great mathematical and computational difficulties emerge in calculation of heat and mass exchange [1]. This is especially evident when the calculation methods used are based on the solution of three-dimensional differential conservation equations for the gaseous atmosphere (GA) of the room with the use of various models of turbulence. Moreover, because of the limited dimensions of a finite-difference grid, these models do not allow one to calculate sufficiently accurately the temperature and velocity fields near open apertures. Therefore, the use of rather simple integral engineering methods of calculation is of practical interest for predicting the dynamics of the dangerous factors of fire (temperature, concentration of combustion products, oxygen, smoke content in GA, etc.) in a room with open apertures. In these methods, the mean volumetric parameters of a GA are calculated, which are used to find the distribution of the corresponding data over the height of the room by means of various formulas [1].

The statement of the problem is given in Fig. 1. Cold air enters the room below the neutral plane (NP), and hot gases filled with smoke flow out through an open aperture above the NP.

2. As the basis of the mathematical model for calculating heat and mass exchange in a room on fire, the integrated model of [1, 3] was taken, in which a number of refinements were made:

a) The heating of the enclosing structures of the room is calculated using the solution of two-dimensional nonstationary heat conduction equations (one-dimensional equations in [1]).

b) The completeness of combustion of the CL is calculated by formulas that take account of the termination of combustion at a low concentration of oxygen in a room (this is ignored in [1]).

c) To calculate the natural gas exchange through an open aperture, the total pressure in the GA (static pressure in [1]) is used, since experimental values of the difference between static pressures indoors and outdoors at the same height have the same order of magnitude with the velocity head in outflowing hot gases (5–10 Pa [1]).

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d) The local coefficients of convective heat transfer are calculated on the outer surfaces of the ES, which is especially important in the case of a thermally "thin" (metallic) ES.

Here, the following basic assumptions were made:

a) There is a good mixing of the combustion products with the entering air over the entire volume of the room.

b) Combustion occurs within the entire volume of the room (volume fire [1]).

c) The character of development of the fire is "quasistationary" (without sharp pressure jumps).

d) The gaseous atmosphere in the room is assumed to be an ideal gas with constant thermophysical properties, since the difference of c_p, R, and k between the combustion products and pure air is small in the temperature range usually observed in fire [1].

The basic equations to calculate heat and mass exchange in the GA of a room on fire have the following form:

a) The mass conservation equation for the GA [1]:

$$V\frac{d\rho_{\rm m}}{d\tau} = \psi + G_{\rm e.o.a} + \rho_{\rm o.a}W_{\rm pl.v} - G_{\rm es.g} - \rho_{\rm m}W_{\rm ex.v} + G_{\rm f.e}\,, \tag{1}$$

where V is the volume of the room; ψ is the rate of gasification of the CL; $G_{\rm e.o.a}$, $G_{\rm es.g}$ are the mass flow rates of the entering and escaping gases in the case of natural gas exchange, respectively; $W_{\rm pl.v}$, $W_{\rm ex.v}$ are the volumetric flow rates in the subsystems of the plenum and exhaust ventilation, respectively; $F_{\rm f.e}$ is the mass flow rate of the fire extinguisher (FE) supplied.

b) The energy balance equation of the GA [1]:

$$\frac{d}{d\tau}\left(\frac{p_{\rm m}V}{k-1}\right) = \psi\eta\,Q_{\rm w}^{\rm low} + c_{p{\rm o.a}}T_{\rm o.a}\,(G_{\rm e.o.a} + \rho_{\rm o.a}W_{\rm pl.v}) + c_{p{\rm f.e}}T_{\rm f.e}G_{\rm f.e} -$$

$$- c_{p{\rm m}}T_{\rm m}\,(G_{\rm es.g} + \rho_{\rm m}W_{\rm ex.v}) - Q_{\Sigma} - Q_{\rm r} + Q_{\rm h}\,, \tag{2}$$

where Q_{Σ} is the overall heat flux in the ES; $Q_{\rm r}$ is the overall heat flux emitted through the apertures; $Q_{\rm h}$ is the heat output into the room from the heating system;

c) The oxygen mass balance equation [1]:

$$V\frac{d\,(X_{\rm O_2m}\,\rho_{\rm m})}{d\tau} = -\,\eta L_{\rm O_2}\psi + X_{\rm O_2o.a}\,(G_{\rm e.o.a} + \rho_{\rm o.a}W_{\rm pl.v}) - X_{\rm O_2m}\,(G_{\rm es.g} + \rho_{\rm m}W_{\rm ex.v})\,. \tag{3}$$

d) The balance equation for the combustion products [1]:

$$V\frac{d\,(X_{i{\rm m}}\,\rho_{\rm m})}{d\tau} = L_i\,\psi - X_{i{\rm m}}\,(G_{\rm es.g} + \rho_{\rm m}W_{\rm ex.v})\,, \tag{4}$$

with the assumption that the air consists only of oxygen and nitrogen.

e) The balance equation for the mass of the combustible material [1]:

$$\frac{dM}{d\tau} = -\,\psi\,, \tag{5}$$

where M is the residual mass of the combustible material.

f) The balance equation of the mass of the inert gas used as the FE [1]:

$$\frac{d\,(\rho_{\rm m}X_{\rm f.e.m}V)}{d\tau} = X_{\rm f.e.o.a}\,(G_{\rm e.o.a} + \rho_{\rm o.a}W_{\rm pl.v}) - X_{\rm f.e.m}\,(G_{\rm es.g} + \rho_{\rm m}W_{\rm ex.v}) + G_{\rm f.e}\,. \tag{6}$$

g) The equation of state of the GA in the room:

$$p_m = \rho_m R_m T_m . \tag{7}$$

The parameters of the exchange of the natural gas between the GA of the room and the environment are calculated from the following formulas [3]:

a) The mass flow rate of the air flowing into the room:

$$G_{e.o.a} = \frac{2}{3}\sqrt{2g\rho_{o.a}(\rho_{o.a} - \rho_m)}\,\xi b\,[\,|Y^* - Y_{low}|^{1.5} - |Y^* - Z|^{1.5}] . \tag{8}$$

b) The mass flow rate of combustion products flowing out of the room:

$$G_{es.g} = \frac{2}{3}\sqrt{2g\rho_m(\rho_{o.a} - \rho_m)}\,\xi b\,[\,|Y^* - Y_{up}|^{1.5} - |Y^* - Z|^{1.5}] , \tag{9}$$

where Y^* is height of the neutral plane (NP); Y_{low}, Y_{up} are the heights from the level of the floor to the lower and upper cuts of the aperture, respectively; ξ is the coefficient of hydraulic resistance of the aperture; b is the width of the aperture.

The height of the NP is

$$Y^* = h - \frac{p_m^* - p_{o.a}}{g(\rho_{o.a} - \rho_m)} , \tag{10}$$

where h is half the height of the room; p_m^* is the total pressure (in contrast to [1]), which is defined in terms of the static pressure of the GA and the velocity head near the open aperture.

The parameter Z is equal to

$$Z = \begin{cases} Y_{low} & \text{when } Y^* \le Y_{low} , \\ Y^* & \text{when } Y_{low} < Y^* < Y_{up} , \\ Y_{up} & \text{when } Y^* \ge Y_{up} . \end{cases} \tag{11}$$

The mass rate of the gasification of a liquid CL is

$$\psi = \psi_{sp} F_f \sqrt{\tau/\tau_{st}} , \tag{12}$$

where ψ_{sp} is the specific mass rate of gasification of the CL; F_f is the fire area of the CL; τ_{st} is the time of stabilization of the combustion of a liquid CL.

In [1], to calculate the completeness of combustion of a CL, an experimental relation is obtained which is valid in the range of mean-volumetric mass concentrations of oxygen of from 0.105 to 0.23:

$$\eta = 0.63 + 0.2X_{O_2m} + 1500X_{O_2m}^6 . \tag{13}$$

To calculate the completeness of combustion of a CL, it is also suggested to use the following formulas that correspond to linear and quadratic dependences on the mean-volumetric mass concentrations of oxygen in the room, respectively:

$$\eta = \eta_{o.a}\overline{X} , \tag{14}$$

$$\eta = \eta_{o.a}(2\overline{X} - \overline{X}^2) , \tag{15}$$

where $\eta_{o.a} = 0.9$ is the completeness of combustion in open air [1], $\overline{X} = (X_{O_2m} - X_{O_2min})/(X_{O_2o.a} - X_{O_2min})$, X_{O_2min} is the concentration of oxygen after the termination of combustion.

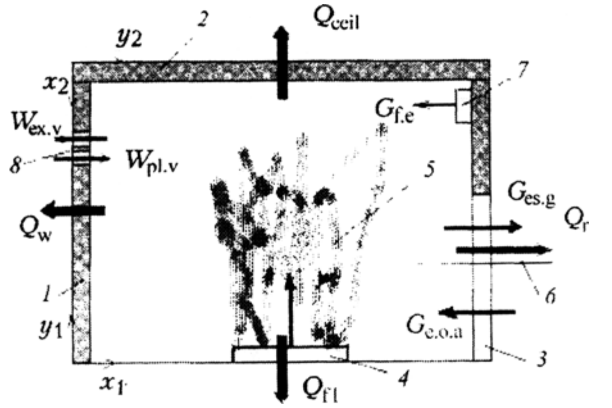


Fig. 1. Basic diagram of the statement of the problem: 1) walls; 2) ceiling; 3) open aperture; 4) combustible material; 5) site of combustion; 6) neutral plane; 7) system of fire-fighting; 8) mechanical plenum-exhaust ventilation.

Heat fluxes released into the ES are calculated as

$$Q_\Sigma = Q_w + Q_{ceil} + Q_{fl} = \alpha_w \int_{F_w} (T_m - T_w)\, dF + 1.7\alpha_{ceil} \int_{F_{ceil}} (T_m - T_{ceil})\, dF , \tag{16}$$

where the coefficients of heat transfer that take into account the joint effect of radiant and convective heat exchange between the GA of the room and the ES are determined from the semiempirical relations [3]:

$$\alpha_w = 15.9\psi^{0.222} , \tag{17}$$

$$\alpha_{ceil} = 17.2\psi^{0.222} / [1 - 0.127\psi^5 \exp(-1.6\psi)] . \tag{18}$$

The heating of the ES is calculated using two-dimensional nonstationary equations of heat conduction written separately for the walls and the ceiling:

$$\rho_w c_w = \frac{\partial T_w}{\partial \tau} = \frac{\partial}{\partial x_1}\left[\lambda_w \frac{\partial T_w}{\partial x_1}\right] + \frac{\partial}{\partial y_1}\left[\lambda_w \frac{\partial T_w}{\partial y_1}\right] , \tag{19}$$

$$\rho_{ceil} c_{ceil} = \frac{\partial T_{ceil}}{\partial \tau} = \frac{\partial}{\partial x_2}\left[\lambda_{ceil} \frac{\partial T_{ceil}}{\partial x_2}\right] + \frac{\partial}{\partial y_2}\left[\lambda_{ceil} \frac{\partial T_{ceil}}{\partial y_2}\right] , \tag{20}$$

where the axes are shown in Fig. 1.

The boundary conditions for Eqs. (19)-(20) have the form:

a) The boundary conditions of the third kind for the inner surfaces of the ES (the heat transfer coefficients are defined by Eqs. (17)-(18), the mean volumetric temperature is T_m).

b) The boundary conditions of the third kind for the outer surfaces of the ES (the heat transfer coefficients are determined from formulas for free convection and radiative heat transfer to the surrounding medium [1], and the ambient temperature is $T_{o.a}$).

c) The boundary conditions of the second kind for the surfaces of contact of the ES with one another (a thermally insulated wall, $q = 0$).

Equations (1)-(20) completely describe the heat and mass exchange in a room on fire and the temperature fields in the ES. This system of differential equations is a "rigid" one [4], and the use of standard Runge–Kutta-type numerical methods for its solution is ineffective, since the step of numerical calculation in time is on the order of 10^{-8} sec. Therefore, a special scheme of numerical calculation of the problem was developed which had a time

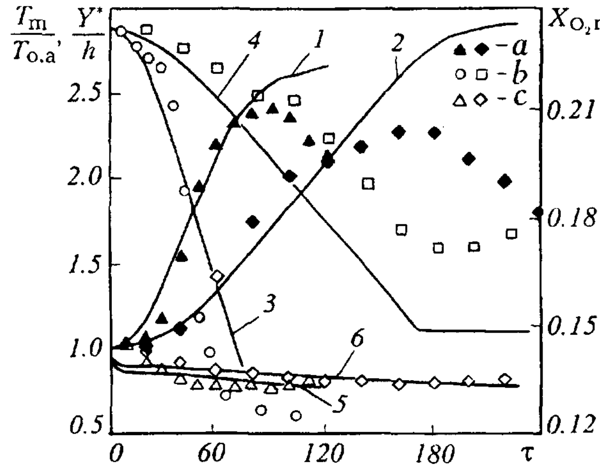


Fig. 2. Dependence of the parameters of the GA of the room on the time of combustion of wood on fire: calculation (1, 2) $T_m/T_{o.a}$; 3, 4) X_{O_2m}; 5, 6) Y^*/h) and experiment [1] (a) $T_m/T_{o.a}$; 6) X_{O_2m}; c) Y^*/h). τ, sec; the remaining quantities are dimensionless.

step of the order of 1–5 sec. Moreover, when $\tau = 0$, the densities of the surrounding air and of the GA are equal to each other. Therefore, in Eq. (10) the denominator of the fraction is also equal to zero. To eliminate this difficulty, special mathematical measures were undertaken.

3. The initial data for a numerical experiment were the following:

a) The room had dimensions of $6 \times 10 \times 2.8$ m.

b) The dimensions of the open aperture (door) were a width of 2 m and a height of 2 m.

c) ES were of two variants: concrete 0.3 m thick and steel 0.03 m thick.

d) CL (kerosene) of mass 500 kg was spread on the floor over an area of 16 m^2.

e) The temperature of the outside air was $T_{o.a} = 293$ K, the pressure $p_{o.a} = 10^5$ Pa.

f) The height of the working zone was 1.5 m.

It was assumed that the systems of forced plenum-exhaust mechanical ventilation, heating, and of fire-fighting were shut off.

The principal parameters of the problem changed in the following ranges:

a) The volume of the room from 90 to 1800 m^3.

b) The area of the open surface of the kerosene from 2 to 32 m^2.

c) The width of the open aperture from 1 to 6 m.

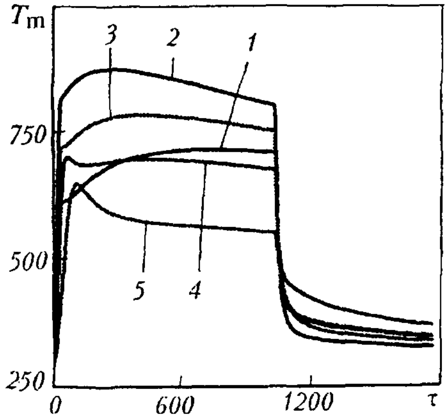
d) The height of the open aperture from 1 to 3 m.

e) The coefficient of heat transfer ranged from 10 to 70 W/(m$^2 \cdot$K), which corresponded to the experimental data of [1].

f) The time for stabilization of combustion was assumed equal to 120, 600, and 1200 sec.

4. The results of a comparison of the computed mean volumetric temperature of the GA in the room, of the height of the NP, and of the mean volumetric concentration of oxygen in the GA with the experimental data of [1] (combustion of wood) are presented in Fig. 2. It is seen from the figure that the agreement of the calculation with experiment is satisfactory for the engineering method of calculation. The substantial difference in the maximum calculated and experimental temperatures is explained by coking of the wood, which is not taken into consideration in the model proposed. However, this phenomenon is not observed in combustion of kerosene. It is also necessary to note that if in formula (10) the static pressure is used instead of the total pressure (as in [1, 3]), the height of the NP exceeds the corresponding calculated values (curves 5 and 6) by 15–20%, i.e., the discrepancy with experiment is larger.

The effect of the coefficient of heat transfer from the GA to the inner surface of the ES and of the room on the mean volumetric temperature is shown in Fig. 3, from which it is seen that the difference of temperatures can be on the order of 200 K.



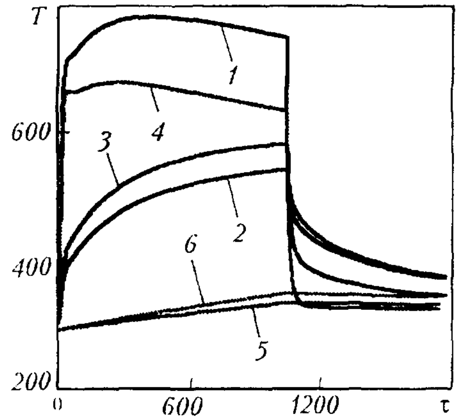


Fig. 3. Dependence of the mean volumetric temperature of the GA of the room on the time of fire: 1) $\alpha_w = \alpha_{ceil} = \alpha_{fl} = 10$ W/(m$^2\cdot$K); 2) $\alpha_w = \alpha_{ceil} = \alpha_{fl} = 70$ W/(m$^2\cdot$K); α_w and α_{ceil} according to Eqs. (16)-(17); V, m^3; 3) 168; 4) 336; 5) 1800. T_m, K; τ, sec.

Fig. 4. Dependence of temperatures on the time of fire at $\tau_{st} = 600$ sec; concrete ES (1) T_m; 2) T_w; 3) T_{ceil}) and steel ES (4) T_m; 5) T_w; 6) T_{ceil}). T_w, T_{ceil}, K.

The calculated dependences of this temperature and of the temperatures of the inner surfaces of the walls at the level of the working zone and ceiling on time for concrete and steel ES are given in Fig. 4. It is seen from the figures that these temperatures depend substantially on the thermophysical properties of the ES material.

The calculations carried out showed that virtually all the parameters of the problem exert a substantial effect on the mean volumetric temperature of the GA and the temperature of the inner surfaces of the ES.

The thermophysical properties of the ES material, the time needed to stabilize combustion, the rate of gasification of the NP, the coefficient of heat transfer from the GA to the inner surface of the ES, the width of the aperture, the completeness of combustion, and the volume of the room exert a weak (not exceeding 10%) effect on the height of the NP during the process of combustion and after its termination. For example, with different formulas used to calculate the completeness of combustion 60 sec after the beginning of the fire, the height of the NP was:

$Y^* = 0.73$ m $-$ $\eta = 0.9$, $T_m = 1060$ K;
$Y^* = 0.77$ m $-$ calculation by (15), $T_m = 880$ K;
$Y^* = 0.79$ m $-$ calculation by (13), $T_m = 748$ K;
$Y^* = 0.80$ m $-$ calculation by (14), $T_m = 453$ K.

From the data presented it is seen that with an increase in the mean volumetric temperature of the GA by a factor of 2.34, the height of the NP decreased by a factor of 1.1.

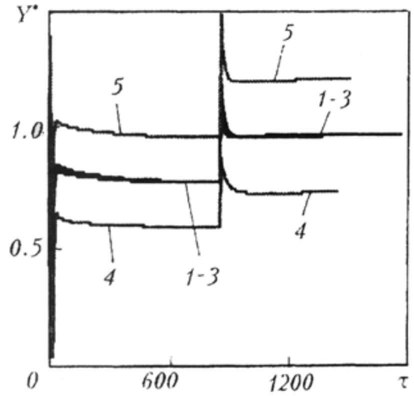
With a change in the volume of the room from 90 to 1800 m^3, 180 sec after the beginning of combustion $Y^* = 0.8$ m for the smaller volume and $Y^* = 0.86$ m for the larger one.

Only the coordinate of the upper edge of the open aperture from the level of the floor exerts a substantial effect on the height of the NP (Fig. 5). Calculations showed that the height of the NP changes little during combustion and after its termination, whereas after complete burning out of a CL it is increased by no more than 25%, and it also virtually does not change for a long time. To calculate the position of the NP, the following formulas were obtained that approximate the results of numerical experiment with an error not exceeding 10%:

a) during fire:

$$Y^* = 0.4Y_{up}; \tag{21}$$

b) after termination of fire:



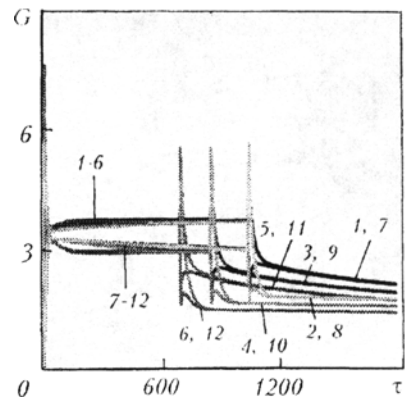
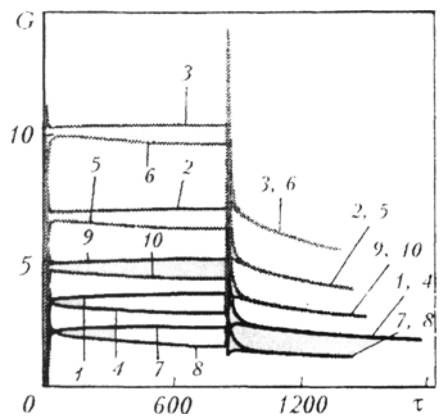


Fig. 5. Effect of dimensions of open aperture on the height of the NP for concrete ES and τ_{st} = 600 sec; b, m (at Y_{up} = 2 m): 1) 2; 2) 4; 3) 6; Y_{up}, m (at b = 2 m): 4) 1.5; 5) 2.5. Y^*, m.

Fig. 6. Dependence of mass flow rates of inflowing air and escaping combustible gases on time at different times of the stabilization of combustion: concrete ES (τ_{st} = 1200 sec; 1) $G_{es.g}$, 7) $G_{e.o.a}$; τ_{st} = 600 sec; 3) $G_{es.g}$, 9) $G_{e.o.a}$; τ_{st} = 120 sec; 5) $G_{es.g}$, 11) $G_{e.o.a}$) and steel ES (τ_{st} = 1200 sec; 2) $G_{es.g}$, 8) $G_{e.o.a}$; τ_{st} = 600 sec; 4) $G_{es.g}$, 10) $G_{e.o.a}$; τ_{st} = 120 sec; 6) $G_{es.g}$, 12) $G_{e.o.a}$). $G_{es.g}$, $G_{e.o.a}$, kg/sec.



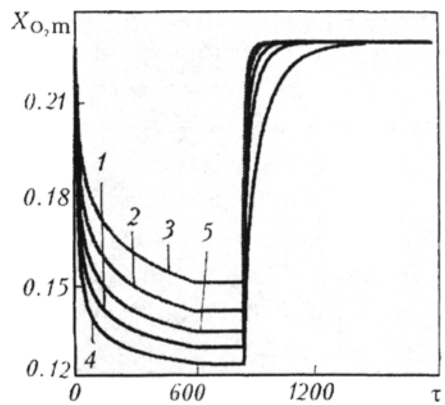


Fig. 7. Effect of the dimensions of open aperture on the mass flow rates of inflowing air and escaping hot gases for concrete ES and τ_{st} = 600 sec; $G_{es.g}$ at b, m (Y_{up} = 2 m): 1) 2; 2) 4; 3) 6; $G_{e.o.a}$ for b, m (Y_{up} = 2 m); 4) 2; 5) 4; 6) 6; Y_{up} = 1.5 m (b = 2 m); 7) $G_{es.g}$; 8) $G_{e.o.a}$; Y_{up} = 2.5 m (b = 2 m); 9) $G_{es.g}$; 10) $G_{e.o.a}$,$G_{es.g}$, $G_{e.o.a}$, kg/sec.

Fig. 8. Effect of the dimensions of open aperture on the mean volumetric mass concentration of oxygen in room with concrete ES and τ_{st}= 600 sec; b, m (at Y_{up} = 2 m): 1) 2; 2) 4; 3) 6; Y_{up}, m (at b = 2 m): 4) 1.5; 5) 2.5. X_{O_2m} is dimensionless.

$$Y^* = 0.48 Y_{up} . \tag{22}$$

Figure 6 presents time dependences (after the start of the fire) of the mass flow rate of the cold air entering the room (curves 1-6) and the mass flow rate of the hot gases leaving the room (curves 7-12) at various magnitudes of the time of stabilization of combustion and different properties of the material of the ES. It is clear that the values indicated above exert a weak effect on the natural gas exchange of the GA of the room with the environment. Similarly, calculation indicates that the coefficient of heat transfer from the GA to the inner surface of the ES, the volume of the room, and the completeness of combustion virtually do not affect the flow rates indicated above.

The coordinates of the lower and upper edges of the aperture from the level of the floor and the width of the aperture (Fig. 7) exert a substantial effect on natural gas exchange.

Calculations showed that only the completeness of combustion, the rate of gasification, and the coordinates of the edges of the aperture from the level of the floor and its width exert an effect on the magnitude of the mean volumetric mass concentration of oxygen. The coefficient of heat transfer from the GA to the inner surface of the ES and the dimensions of the room virtually do not affect $X_{O_2 m}$. The effect of the dimensions of the open aperture on the mean volumetric mass concentration of oxygen in the room is shown in Fig. 8.

The remaining dangerous factors of the fire, such as the mean volumetric mass concentrations of carbon monoxide and carbon dioxide and other combustion products behave similarly, since their magnitudes are described by similar differential equations (4).

CONCLUSIONS

1. In combustion of a liquid CL in a room, the natural gas exchange between the GA and environment through open apertures substantially depends only on the coordinates of the lower and upper edges of the apertures from the level of the floor and on their width. Here the height of the NP is virtually independent of the width of the aperture.

2. All of the above-considered parameters of the problem exert a noticeable effect on the mean volumetric temperature of the GA and the temperature fields in the ES.

3. The thermophysical parameters of the ES of the room do not affect natural gas exchange or mean volumetric mass concentrations of oxygen and combustion products in a room on fire, but considerably influence the mean volumetric temperature of the gaseous atmosphere of the room and the temperature fields in the ES.

4. The mean volumetric mass concentrations of oxygen and combustion products in the GA of the room substantially depend only on the coordinates of the lower and upper edges and on the width of the apertures from the level of the floor, the completeness of combustion, and the rate of gasification of the liquid CL.

NOTATION

T, temperature; ρ, density; c_p, isobaric specific heat; c, specific heat; τ,time; p, pressure; k, specific heat ratio of the GA; R, gas constant; F, area; α, heat transfer coefficient; λ, heat conduction coefficient; Q, heat flux; $Q_{\mathrm{w}}^{\mathrm{low}}$, lower working heat of combustion of CL; η, completeness of combustion; q, specific heat flux; X, mean volumetric mass concentration of gas in room; L_{O_2}, quantity of oxygen needed burn 1 kg of CL; L_i, specific mass liberation of the i-th product of combustion; G, mass flow rate of gas; W, volumetric flow rate of gas. Subscripts: m, mean volumetric parameters of GA in room; o.a, outside air; f.e, FE; O_2, oxygen; w, walls; ceil, ceiling; fl, floor; low, lower edge of aperture; up, upper edge of aperture; sp, specific parameters; e.o.a, entering outside air; es.g, escaping gases; pl.v, plenum ventilation; ex.v, exhaust ventilation; min, minimum value; st, stabilization of combustion; h, heating system; r, radiation through aperture; Σ, overall heat flux.

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