Numerical method for fire simulation in a working premise

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The numerical method is essential when it is necessary to solve problems based on thorough knowledge of physical picture of fife. The quoted results and empirical tests in this sphere characterize quite well the overall picture of how fire spreads.

Through numerical method and mathematical modeling we get the idea of the values, distribution and the rate of change of basic and critical parameters which should be taken into consideration in fire safety design of buildings and installations and as well in firefighting and evacuation of people and property.

Field of application

The approximate model for numerical study has its own importance in clarifying the characteristics of the upward convection current. The quoted results of numerical study confirm very well its relevance to the purposes of fire safety and ecology.

Mathematical model - Numerical solution (research)

The methodology of the mathematical model contains a closed system of equations which can be solved only by numerical method. Present day development of computing technologies (machines) and computational mathematics gives the opportunity to work out a sufficiently accurate numerical method in which extremely different schemes of initial systems of equations are applied. The numerical method for solution of a system of differential equations in private derivatives is applied – "Volume control" method. This method is used in modern software packages for solving practical problems of gas dynamics, heat and mass transfer - PHOENICS and FLUENT.

The above mentioned method is used to solve: 3D differential equations representing the law of the mass, momentum and energy conservation in gas medium in a premise; the equations of gas components mass conservation and the optical density equations. All differential equations are reduced to a "standard" form - convenient for numerical solutions:

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

where: **Φ** - - dependent variable (of the enthalpy of the gas mixture and of wall materials and coatings, the projection of velocity on a coordinate axis, the content of gas components in the mixture, the kinetic energy of turbulence, and according to their rate of dissipation, mass concentration and optical density of smoke);

Γ – diffusion coefficient of Φ;

S – number of sources of Φ;

The values in the equation are given in the table. All quantities are averaged over time. When calculating heating and enclosing structures:

w_x=w_f=w_z=0.

X_{O2}, X_{CO}, X_{CO2}, X_{N2}, X_{H2O}, $X_{пг}$ – Mass concentrations of oxygen, carbon monoxide, carbon dioxide, nitrogen, water and combustion products

D_{O2}, D_{CO}, D_{CO2}, D_{N2}, D_{H2O}, $D_{пг}$ – Difusion coefficients of oxygen, carbon monoxide, carbon dioxide, nitrogen, water and combustion products [m^2/s]

m_{O2}, m_{CO}, m_{CO2} – Intensity of absorption of the inner mass of oxygen, carbon monoxide, carbon dioxide as a result of the formation (disappearance) of molecules of a given gas flow as a result of the chemical reaction in the combustion, kg/(s . m^3);

***m_{H2O}* –** Intensity of absorption of the inner mass of water (water vapor) as a result of evaporation (condensation) under the influence of the room temperature and enclosing structures (walls and ceilings), kg/(s . m^3)

β = 1/*T* – Volumetric thermal expansion coefficient, 1/K;

***LO2* –** Mass of oxygen necessary for burning of one kilogram of combustible material

***LCO, LCO2* –** Mass of carbon monoxide, carbon dioxide released by burning of one kilogram of combustible material;

Ψг – Burning rate of the combustible material, kg/s

***D*опг –** Smoke producing capacity of burning material , Нп . m^2/kg

***i, i_w, i_c* –** Enthalpy of: gas mixture, material and of the walls and floors, J / kg

***Q*р^{н} –** The lowest operating heat by combustion, J / kg

η- Burning efficiency;

***q_D* –** Intensity of the internal sources of optical smoke density formed as a result of combustion reactions, Hn / (sm)

qvw, qvc - Intensity of the internal heat source in the walls and floors, W / m3;

Δ*V* – Volume of gaseous medium which is located inside the power source m3;

Table 1 Parameters and coefficients:

№	Ф	Г	S
1	1	0	0
2	w_x	μ + $μ_T$	$\frac{\partial}{\partial x}\left(\Gamma\frac{\partial w_x}{\partial x}\right)+\frac{\partial}{\partial y}\left(\Gamma\frac{\partial w_y}{\partial x}\right)+\frac{\partial}{\partial z}\left(\Gamma\frac{\partial w_z}{\partial x}\right)-\frac{\partial p}{\partial x}-\frac{2}{3}\frac{\partial}{\partial x}(\Gamma\mathrm{div}\mathbf{w})$
3	W_y	μ + $μ_T$	$\frac{\partial}{\partial x}\left(\Gamma\frac{\partial w_x}{\partial y}\right)+\frac{\partial}{\partial y}\left(\Gamma\frac{\partial w_y}{\partial y}\right)+\frac{\partial}{\partial z}\left(\Gamma\frac{\partial w_z}{\partial y}\right)-\frac{\partial p}{\partial y}-\frac{2}{3}\frac{\partial}{\partial y}(\Gamma\mathrm{div}\mathbf{w})$
4	W_z	μ + $μ_T$	$\frac{\partial}{\partial x}\left(\Gamma\frac{\partial w_x}{\partial z}\right)+\frac{\partial}{\partial y}\left(\Gamma\frac{\partial w_y}{\partial z}\right)+\frac{\partial}{\partial z}\left(\Gamma\frac{\partial w_z}{\partial z}\right)-\frac{\partial p}{\partial z}-\frac{2}{3}\frac{\partial}{\partial x}(\Gamma\mathrm{div}\mathbf{w})-\beta g\Delta T$
5	X_{O2}	$(D_{O2}+ D_T)ρ$	$mO2 = L_{O2}Ψrη/ΔV$
6	X_{CO}	$(D_{CO}+ D_T)ρ$	$mCO = L_{CO}Ψrη/ΔV$
7	X_{CO2}	$(D_{CO2}+ D_T)ρ$	$mCO2 = L_{CO2}Ψrη/ΔV$
8	X_{N2}	$(D_{N2}+ D_T)ρ$	0
9	X_{H2O}	$(D_{H2O}+ D_T)ρ$	m_{H2O}
10	$X_{пг}$	$(D_{пг}+ D_T)ρ$	$m_{пг}$
11	$D_{оп}$	0	$q_D = D_{опг}Ψr/ΔV$
12	i_w	$λ_w$	q_{vw}
13	i_c	$λ_c$	q_{vc}
14	i	$λ + λ_T + λ_Л$	$Ψrη Q ρ^{н}/ΔV - q_{vp}$

The partial differential equations, transformed to "standard" type are solved with the best tested implicit method - "volume control". For three-dimensional problems the discrete analogue of the equation has the following form:

$$a_pΦ_p = aEΦE + aWΦW + aNΦN + a_sΦ_s + aTΦT + aBΦB + b, \quad (2)$$

where: $a_E = D_EA(|P_E|) + [|-F_E,0|]$; $a_N = D_NA(|P_N|) + [|-F_N,0|]$; $a_T = D_TA(|P_T|) + [|-F_T,0|]$; $a_W = D_WA(|P_W|) + [|F_W,0|]$; $as = DsA(|Ps|) + [|Fs,0|]$; $a_B = D_BA(|P_B|) + [|F_B,0|]$;

points ***T*** and B are similarly positioned in ***YOZ*** and ***XOZ*** planes;

$$a_p = a_E + a_W + a_N + a_S + a_T + a_B + a^0{}_p - S_pΔxΔyΔz;$$

$$b = S_CΔxΔyΔz + a^0{}_pΦ^0{}_p;$$

ρ^0_p – value of density at an earlier moment kg/m3; Φ^0_p – value of the function at an earlier moment; ***Δx, Δy, Δz*** – intervals (changes) along the relevant axes ***OX, OY, OZ***, m; ***Δτ*** – time interval, s.

The gradient model of turbulence - k-ε model is the most fully developed and commonly used model for determining the heat and mass transfer in a fire. It is assumed, in this model, that the coefficient of turbulent viscosity is dependent on the turbulence kinetic energy and its dissipation rate in accordance with Kolmogorov's formula:

$$v_T = C\mu\frac{k^2}{\varepsilon} \tag{3}$$

where: v and $v_т$ are cinematic coefficients of molecular and turbulent viscosity, espectively, m^2/s;

$k = \frac{1}{2}\left(\overline{w_x'^2} + \overline{w_y'^2} + \overline{w_z'^2}\right)$ - turbulent kinetic energy m^2/s^2

w'_x, w'_y, w'_z – Velocity pulsations projected on the relevant axes, m/s; $C_\mu = 0{,}09$ - empirical constant;

$\varepsilon = \nu\left(\overline{\left(\frac{\partial w'_x}{\partial x}\right)^2 + \left(\frac{\partial w'_y}{\partial y}\right)^2 + \left(\frac{\partial w'_z}{\partial z}\right)^2}\right)$ - dissipation rate of the turbulence kinetic energy– m^2/s^3

The coefficient of dynamic molecular viscosity of the gas is determined by the value of the kinematic molecular viscosity calculated using Sezerlend's formula:

$$\frac{\mu}{\mu_0} = \frac{1+\frac{C}{T_0}}{1+\frac{C}{T}}\sqrt{\frac{T}{T_0}} \tag{4}$$

където : C – empirical constant for the particular gas, K; μ – coefficient of dynamic molecular viscosity kg/(m · s); μ_0 – known value of the dynamic viscosity at a selected temperature T_0, kg/(m · s).

The values of C and T_0 are taken from construction guides (In present study S.S. Kutateladze's "Basics of heat transfer theory", M. Atomizdat, 1979 is used.)

Considering that in fire the density of the gas environment in the premise changes substantially, it is necessary to use an equation to determine a correction for the pressure in the "compressible" shape

$$a_p p'_p = a_E p'_E + a_W p'_W + a_N p'_N + a_S p'_S + a_T p'_T + a_B p'_B + b, \tag{5}$$

where: $p'i$ – correction of pressure in the particular point.

The correction formulas for projections of velocity are:

$$w_{xe} = w^*_{xe} + d_e(p'_p + p'_E); \tag{6}$$

$$w_{yn} = w^*_{yn} + d_n(p'_p + p'_N); \tag{7}$$

$$w_{zt} = w^*_{zt} + d_t(p'_p + p'_T), \tag{8}$$

where: the quantities with superscript '*' are their current values and these with index' ' ' – the corrected values; ***de, dn, dt*** - values obtained from the relevant equations for velocity components.

The calculation is performed on separate highly different spatial grids with variable steps (Δx = var, Δy = var, Δz = var) as determined by Courant's condition for all points of the different grids:

$$\Delta\tau = k_\tau min\left(\frac{\Delta x}{w_a + |w_x|}, \frac{\Delta y}{w_a + |w_y|}, \frac{\Delta z}{w_a + |w_z|}\right) \tag{9}$$

where: wa – local speed of sound, m/s, $k_т < 1$ - **Courant** number.

An indirect radically different scheme is used. This system of linear algebraic equations (2) is solved by the longitudinal-transverse sweep method. First, a solution is

done at one of the selected direction (e.g., toward the OX axis) by the method of Gauss. Each equation of the system has the following form:

$$a_i\Phi_i = b_i\Phi_i{+}1 + c_i\Phi_i{-}1 + d_i, \quad (10)$$

where: $i = 1, 2, ..., Nx$ – number of the point in the radically different scheme toward OX axis. In this case, the physical quantity Φi is related to the adjacent key values Fi-1 and Fi + 1. It is assumed that there is the following relationship:

$$\Phi_i = \alpha_i\Phi_i{+}1 + \beta_i, \quad (11)$$

where: α_i и β_i – are correction coefficients.

By replacing (11) in (10), we receive the relationship of correction coefficients α_i and β_i with $\alpha_i{-}1$ and $\beta_i{-}1$:

$$\alpha_i = \frac{b_i}{a_i - c_i\alpha_{i-1}} \quad (12)$$

$$\beta_i = \frac{d_i + c_i\beta_{i-1}}{a_i - c_i\alpha_{i-1}} \quad (13)$$

The meanings of α_i and β_i are defined by the boundary conditions:

$$\alpha_i = b_i/a_i;\ \beta_i = d_i/a_i. \quad (14)$$

For example, in the case of second type boundary conditions and projecting to the axis OX, energy equation is:

$$q = \lambda\left(\frac{\partial T}{\partial n}\right)_c \approx \lambda\frac{T_1 - T_1}{\Delta x} \quad (15)$$

where: $\left(\frac{\partial T}{\partial n}\right)_c$ is the temperature gradient along the normal to the surface of the surrounding construction; T_1, T_2 – temperatures in the middle of the border and the adjacent control volumes. Δx – move along ***OX axis***.

Then, in accordance with equations (11) and (15) the values of αi and βi are equal:

$$T1 = \alpha_i T2 + \beta_i = q\Delta x/\lambda + T2;\ \alpha_i = 1;\ \beta_i = q\Delta x/\lambda. \quad (16)$$

After that all correction coeffiecients are calculated using the formulas (12) and (13).

Moreover, using the boundary conditions at other border ($i = Nx$) the value ΦNx is determined and using formula (11) all others Φi are determined. For example, in case of second type boundary conditions, in the case of a correction to the axis OX, the energy equation is:

$$T_{Nx-1} = \alpha_{Nx-1}T_{Nx} + \beta_{Nx-1} = q\Delta x/\lambda + T_{Nx}; \quad (17)$$

where: T_{Nx}, T_{Nx-1} - the temperatures in the middle of the border and the adjacent control volumes;

CONCLUSION

Similar corrections to the other two axes OY and OZ are done using the values of Φi obtained from the last iteration. The described algorithm is repeated to all axes as long as the values of Φi from the previous and the successive iteration, in all nodes of the radically different grid, differ by a predetermined value.

Intricate geometric structure and bulky objects block some hard surface into the control volume of the radically different scheme (network) grid used for numerical solution of a computer model which predetermines too high viscosity of the gas mixture: $\mu = 10^{14}$ kg/(m · s).

Literature

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