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MATHEMATICAL MODELLING OF CONCENTRATION PATTERNS OF HARMFUL SUBSTANCES DURING THE PRODUCTION OF BUILDING MATERIALS

Statement of the problem. The existing methods do not always allow one to estimate the allocation of harmful substances in the production of building materials, therefore the problem of the development of mathematical models of the concentration patterns of hazardous substances and its use for environmental safety assessment is important. The approach to numerical modelling of processes of ventilation consists of construction and numerical analysis of a set of equations based on the equations of a mechanics of continuous environments and the algorithms for their solution using the modern information technology is proposed.

Results. The mathematical model of transfer processes of the harmful substances, including the continuity equations, Navier-Stokes, the equations of k-ε turbulence models, a transfer equation of heat and a transfer equation of a hazardous substance with applicable initial and boundary conditions is elaborated. The mathematical model is implemented in the form of programs in the environment of package MatLab in a combination with a programming language C ++.

Conclusions. The outcomes obtained by means of the mathematical models of processes of ventilation, allow one to estimate the effect of various factors on the process of forming of fields of velocities, temperatures of air streams and concentration of hazardous substances and based on that, to improve the effectiveness of the systems of organizing a microclimate. The outcomes obtained using the model will enable a choice of the effective scheme and magnitude of an air exchange for facilities with outtake streams and convection streams and with the emission of hazardous substances lighter and heavier than air.

Keywords: mathematical modelling, environmental safety.

Introduction

At the centre of the design of ventilation systems is the information on heat mass exchange taking place in ventilated premises and generating velocity fields, air temperatures and concentrations of harmful substances.

The parameters of the air environment are significantly affected by air flows propagating in premises, building structures, input ventilation flows, sources of heat and harmful substances.

The understanding of the laws of the development of the parameter fields can be used to create them in premises of necessary parameters of the air environment.

The approach to numerical modelling of ventilation processes involves designing and analyzing numerically systems of equations based on a continuity equation and their solution algorithms making use of modern information technologies.

From the point of view of mathematical modelling ventilation processes take place in a three-dimension space of a complex shape with input-output holes to supply and remove the air and technological equipment to emit heat and harmful substances. In a three-dimension space there is the air moving at significantly ultrasonic speeds at the numbers *Maxa* $M \ll 1$. The model of ventilation processes includes non-stationary mass preservation equations, impulse and energy transfer in natural Reynolds averaged variables. Since $M \ll 1$, dynamic compression of the air can be neglected. The major variables are the pressure, air density, temperature, air velocity, enthalpy and concentration of harmful substances.

1. Mathematical model of ventilation processes of the transfer of harmful substances

Let us investigate the major physical processes that generate fields of pressure, velocity, temperature of air flows and concentration fields of harmful substances [1, 3, 9, 10, 12—15, 22—24].

A non-stationary continuity equation in the integral form is

$$\frac{\partial}{\partial t}\int_V \rho dV + \int_S (\rho\vec{u},\vec{n})\, dS = 0, \qquad (1)$$

where t is the time, sec; ρ is the air density, kg/m^3; $\vec{n}$ is a unit vector that is normal in relation to the area surface; $\vec{u}$ is the air velocity vector; V is the integration area, m^3; S is the surface of the integration area, m^2.

A non-stationary differential equation of continuity in partial derivatives is

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i)=0, \qquad (2)$$

where x_i is the *i*-th spatial coordinate, m; u_i is an air velocity component along *i*-th spatial coordinate, m/sec.

The model uses one of the impulse preservation equations applied to model air flows with low velocities and it allows varying densities. The impulse transfer equation in the integral form is

$$\frac{\partial}{\partial t}\int_V \rho \vec{u} dV+\int_S \rho \vec{u}(\rho \vec{u},\vec{n})-\vec{n}\tau dS=\int_S \rho \vec{f} dV, \qquad (3)$$

where τ is the stress tensor; $\vec{f}$ is the mass force vector.

A non-stationary differential equation of the impulse teransfer in partial derivatives is

$$\frac{\partial(\rho u_i)}{\partial t}+\frac{\partial(\rho u_i u_j)}{\partial x_j}=\frac{\partial \tau_{ij}}{\partial x_j}+\rho f_i, \qquad (4)$$

where f_i are the projections of the mass force vector, H.

The equations are made maximum short. However, it becomes rather deliberate if all the members of the equation are extended.

The Newton's law of friction that connects the stress tensor and tensor of deformation velocity of a viscous gas is given by

$$\tau_{ij}=\mu\left(2S_{ij}-\frac{2}{3}\delta_{ij}(\nabla\cdot\bar{u})\right), \qquad (5)$$

$$S_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right), \qquad (6)$$

where *i*, *j* take on values 1, 2, 3; μ is a dynamic viscosity of the air, kg/(m·sec); δ_{ij} is the Kronecker symbol. The member S_{ij} is a symmetrical tensor of relative deformation written down in the accepted tensor form.

Inserting (5) and (6) into (4), we obtain Navier-Stokes equation for the air

$$\frac{\partial(\rho u_i)}{\partial t}+\frac{\partial(\rho u_i u_j)}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\Gamma^u_{eff}S_{ij}\right)-$$
$$-\frac{2}{3}\frac{\partial}{\partial x_i}\left(\Gamma^u_{eff}\frac{\partial u_j}{\partial x_j}\right)-\frac{2}{3}\frac{\partial}{\partial x_i}(\rho k)-\delta_{i3}\rho g, \quad (7)$$

where g is the gravitational acceleration, m/sec^2; Γ^u_{eff} is an effective diffusion coefficient for the variable u, kg/(m·sec).

In order to describe turbulent values, the standard k-ε-turbulence model is used in the model for a mass density of turbulent energy k and dissipation rate of turbulent energy ε. k-ε-model is most commonly used for a wide range of tasks involving a turbulence model.

The transfer rate of kinetic energy of turbulent air ripples is given by

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho u_i k)}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\Gamma^k_{eff}\frac{\partial k}{\partial x_i}\right)+G^k+G^b-\rho\varepsilon, \quad (8)$$

where k is the energy generation rate of turbulent ripples, m^2/sec^2; ε is the dissipation rate of the energy of turbulent ripples, m^2/sec^3:

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\frac{\partial(\rho u_i\varepsilon)}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\Gamma^\varepsilon_{eff}\frac{\partial\varepsilon}{\partial x_i}\right)+\frac{\varepsilon}{k}\left(C_1\left(G^k+G^b\right)-C_2\rho\varepsilon\right), \quad (9)$$

where C_1, C_2 are the constants of the turbulence model; G^k and G^b are given by the ratios

$$G^k=2\mu_t\left(\sum_i\left(\frac{\partial u_i}{\partial x_i}\right)^2\right)+\mu_t\left(\sum_{i>j}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)^2\right), \quad (10)$$

$$G^b=\mu_t g\frac{1}{\rho}\frac{\partial\rho}{\partial x_3}, \quad (11)$$

where μ_t is the turbulent dynamic viscosity of the air, kg/(m·sec):

$$\mu_t=C_\mu\frac{\rho k^2}{\varepsilon}. \quad (12)$$

The effective dynamic viscosity of the air is

$$\mu_{eff} = \mu + \mu_t . \tag{13}$$

The effective diffusion coefficient for a variable Φ:

$$\Gamma_{eff}^{\Phi} = \frac{\mu_{eff}}{\sigma^{\Phi}} , \tag{14}$$

where σ^{Φ} are the constants of the turbulence model for a variable Φ.

The ratio of the dynamic viscosity of the air to the temperature is given by the ratio

$$\mu = \mu_0 \frac{273{,}15 + C_s}{T + C_s} \left(\frac{T}{273{,}15} \right)^{\frac{2}{3}} , \tag{15}$$

where C_s is the constant; μ_0 is the coefficient of the dynamic viscosity under normal conditions, kg/(m·sec).

For the constants of the turbulence model the following values were adopted:

$C_1 = 1,42;\ C_2 = 1,8;\ C_\mu = 0,09;$

$\sigma^k = 1,0;\ \sigma^\varepsilon = 1,1;\ \sigma^u = 1,0.$

The heat transfer equation is

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho u_i h)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\Gamma_{eff}^{h} \frac{\partial h}{\partial x_i} \right) + q , \tag{16}$$

where q is the function of the heat emission by sources, Watt/m^3, which allows the control over the heat emissions in the premises; h is the specific enthalpy of the air, J/kg:

$$h(T) = \int_{T_0}^{T} c_p(T)\, dT , \tag{17}$$

where $c_p(T)$ is the specific mass isobar heat capacity of the air, J/(kg·K); T is the temperature of the air, K.

The equation of the condition of the air is

$$\rho RT = pM \ , \tag{18}$$

where R is a universal gas constant, J/(mole·K); M is the molar mass of the air, kg/mole.

The equation of the transfer of a harmful substance is

$$\frac{\partial\left(\rho c^o\right)}{\partial t}+\frac{\partial\left(\rho u_i c^o\right)}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\Gamma_{eff}^c\,\frac{\partial c^o}{\partial x_i}\right)+m_u\,. \tag{19}$$

where c^0 is a dimensionless concentration of a harmful substance; m_u is the function of the sources of harmful substance emission, kg/(sec·m^3).

In the premises the function of the sources of harmful substance emission m_u is specified which describes a harmful substance penetrating the premises.

2. Initial and boundary conditions of the model. The initial conditions need to be specified for the models with non-stationary ventilation processes

Depending on the type of a ventilation process, at the initial moment at all the points of the design area velocity, pressure, temperature and concentration of harmful substances are specified and they can differ at different points of the area [2, 4—9, 11, 16, 28, 29].

A wide range of initial conditions are possible to use depending on the configuration of a particular premises. The model uses solid and free boundaries.

The boundary conditions on the solid boundaries are determined by

– adhesion conditions;
– conditions of the air slipping in specified for the velocity vector for the solid conditions;
– temperature of the envelope structures;
– heat exchange on the envelope structures;
– mass exchange on the envelope structures.

The boundary conditions on the free boundary are determined by

– pressure values;

- air velocity in the normal to the boundary or at an angle to the normal;
- conditions of the air flowing out with a null pressure gradient;
- temperature of the inflow air;
- concentration of a harmful substance in the input air flows.

The boundary conditions can be specified by the time variables.

A particular choice of initial and boundary conditions depends on the problem at hand.

3. Implementation of a mathematical model

In order to solve the equations of the mathematical model, the finite difference method was employed based on designing a discrete space-time grid, replacing the derivatives in the initial differential equations by the equivalent finite difference expressions and regrouping the members of the obtained algebraic equations in order to design the algorithm for their solution implemented on a PC at a minimum resource cost [17—20, 25—27, 30].

All the spacial derivatives are approximated by second-order finite differences. The variables of the flow are renewed in time using a second-order predictor-corrector scheme.

The mathematical model was implemented in *MatLa*b environment in conjunction with the programming language *C*++. In order to design the software, the internal interface between *MatLab* and *C*++ was used to give access to the built-in mathematical functions of *MatLab* libraries.

Conclusions

The mathematical model was developed of the transfer of harmful substances that included continuity equations, Navier-Stokes equations, equations of the *k*-ε-turbulence model, heat transfer equation and equation of the transfer of a harmful substance with the relevant initial and boundary conditions.

The mathematical model was implemented in *MatLab* environment in conjunction with the programming language *C*++. In order to design the software, the internal interface between *MatLab* and *C*++ was used to give access to the built-in mathematical functions of *MatLab* libraries.

The results obtained with the help of the mathematical models of ventilation processes permit the assessment of the influence of various factors on the formation of velocity fields, temperature of air flows and concentration of harmful substances and improve the microclimate performance based on that.

The model is crucial to the solution of a range of engineering problems involving the ventilation of the building industry with the emission of heat, moisture and harmful substances. The results obtained with the help of the model give an opportunity to make better-informed choices of effective schemes and air exchange for premises with ventilation flows and convective flows with the circulation of harmful substances lighter and heavier than the air and, finally, to improve their environmental safety.

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