RESOURCES AND PROBLEMS OF THE MATHEMATICAL SIMULATING THERMO-TECHNOLOGICAL PROCESSES

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Abstract. The paper presents the combustion of natural gas in a short flame in the entourage of the very hot air which has produced extremely elevated temperature of the flame, reaching 2300...2500 °C at the front of burning. In the stagnant part of the gas space beyond the short flame, the temperature of gases has gone down, approaching gradually to temperature of the molten-glass surface. As it is well known, a relatively low temperature level of the stagnant gas space allows zones of glass cooling to be organized at the end of the molten-glass basin of the glass furnaces with returned gas flow.

The contemporary methods of mathematical simulation allow rendering numerically and graphically the heat-transfer processes in high-temperature thermo-technological plants, what creates new possibilities for their researches. Mathematical models of the processes, executed in fluid medium, are focused on the numerical solving the complicated enough systems of partial differential equations. First of all, such are the Navier-Stokes equations, which numerical solution defines interrelated components of the fluid velocity \( u, v, w \), directed accordingly along axes \( x, y \) and \( z \).

All the three Navier-Stokes differential equations for a steady subsonic flow can be presented in tensorial notations:

\[
\frac{\partial \rho u_i}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} \right) = - \frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial \rho}{\partial x_i} gh,
\]

where \( \rho \) is the fluid density; \( g \) is the gravitational acceleration; \( \mu \) is the dynamic viscosity, \( h \) is a vertical coordinate. The static pressure \( p \) is replaced here with a pressure function \( \tilde{p} \), which introduces the gravity into the equations implicitly and uniformly for all the three coordinate axes [1]:

\[
\tilde{p} = p + \rho gh,
\]

Subscripts \( i \) and \( j \) accept values 1, 2 or 3 according to numbering of the coordinate axes. Besides, the agreement is implemented here that a sum of three terms of an identical structure can be represented in such an equation as one item with any subscript repeated in it.

The pressure function depends immediately on the three velocity components. As a result, a system of the interrelated differential equations would be formed. In order to solve them, the effective numerical double-sweep method has to be supplemented with numerous iterations, in order to specify factors in discrete counterparts of the differential equations.

The numerical solving the equation system becomes more complicated when the turbulent motion of fluid should be simulated. The eddy counterpart \( \nu_e \) of the kinematic viscosity, subject to local values of kinetic energy of turbulence \( k \) and of its dissipation rate \( \varepsilon \), is usually determined with the help of standard turbulence model [2]:

\[
\nu_e = C_\mu \frac{k^2}{\varepsilon},
\]
where $C_i$ is a factor of proportionality.

Values of $k$ and $\varepsilon$ are computed at grid nodes by means of the numerical solution of two transport equations:

$$\frac{\partial \rho u_j k}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ \rho (v + v_e) \frac{\partial k}{\partial x_j} \right] = \rho (G - \varepsilon),$$

$$\frac{\partial \rho u_j \varepsilon}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ \rho \left( \frac{v + v_e}{\sigma_v} \right) \frac{\partial \varepsilon}{\partial x_j} \right] = \rho (c_{\varepsilon} G - c_{\varepsilon 2} \varepsilon) \frac{\varepsilon}{k},$$

where $G$ is a rate of generation of the turbulence energy, which depends on the velocity distribution; $\sigma_v$, $c_{\varepsilon 1}$, $c_{\varepsilon 2}$ are empirical factors.

It should be intended that the computer representation of numbers has a small error of their rounding, which considerably increases amassing in the double-sweep method for totality of grid nodes. Numerical solving applied to the interdependent differential equations of mathematical models results in multiple increasing faults of the computed functions.

For example, inexact values of the velocity that are transferred in the differential equations of the turbulence model increase the inexactness of the eddy viscosity. Since the eddy viscosities have to be summed up with the kinematic ones in the equations (1), the fault of the velocity components would be computed in next iterations at certainly inaccurate values of the eddy viscosity would be augmented. As a result, the iteration convergence might be slowed down or even ceased.

Such an algorithm has been applied to the numerical simulation of haydite calcining in a rotary kiln, whose inner diameter equals 2 m, and the length is 40 m. The manufacturing 7 t/h of haydite consumed 700 m$^3$/h of natural gas at 10% excess of air. A calcined bed was formed in the furnace by wet clay granules, whose humidity mounted to 11%. Air, heated up to 320 °C, was supplied for the fuel combustion through the unoccupied cross-section of the furnace.

Diffusion burning of natural gas was simulated by transport differential equations for the fuel and air concentrations. An additional transport equation for water vapor allowed computing a temperature reduction, produced in consequence of moisture evaporation from raw granules. When calculating temperature of the internal hot surface of the walls, heat fluxes from gases were determined with taking account of convective and radiative transfer. Also the simulation took into consideration the direct radiation of the refractory on the calcined bed in spectral "windows" and sudden changes of the wall temperature at periodic alighting of rotating walls under the bed.

In order to solve numerically the system of twelve differential equations with a personal computer at more than 200,000 grid nodes, it had required to accomplish above 12,000 iterations, what had ensured high accuracy of obtained results.

An image, presented at Fig. 1, adumbrates the temperature field in the kiln gaseous space. An average temperature of granules, which had reached 1200 °C in the heated-up bed, might be evidence of good compliance of the computed thermal conditions with technological requirements for the haydite calcining. Thus, adequate results have been obtained at this mathematical simulation, in spite of the fact that the errors of the numbering slowed down the iteration convergence.

![Figure 1. Computer image of the temperature field at haydite calcining in the rotary kiln](image-url)
Nevertheless, some predicaments can appear sometimes in the computer realizing mathematical models of high-temperature processes. There are an experience of difficult numeric simulating the diffusion burning and heat exchange in a glass furnace, whose length was 5.2 m and width 3 m. Fig. 2 offered a view on its front wall with two rectangular windows for inputting hot air and removal of gases. A longitudinal section of furnace, which is also presented there, gives an idea about a complicated form of the computational domain.

The natural gas was supplied at a rate of 180 m$^3$/h and velocity of 102 m/s through a nozzle diameter of 25 mm in an inlet air duct, whose lower part constitutes a peculiar fire-chamber of 600 mm in length. The fuel nozzle is inclined up at angle 5°. The arch of the air duct is established at angle 25° to the horizontal; because of that, a current of the air, which had been heated up in a regenerator to 1000 °C, got an impulse directed down to a molten-glass basin.

![Figure 2](image)

**Figure 2.** Outline of the glass furnace on the monitor screen for inputting initial data of the numeric experiment

A problem of choosing and applying the turbulence model that would be efficient enough became especially acute at the numerical simulating the fuel burning in the furnace. The standard turbulence model did not assure the iteration convergence involving the system of interdependent equations for such an intricate flow of high-temperature gases. Calculation errors of the eddy viscosity produced by the formula (2) brought, finally, to unduly big fluctuations in computable values of the velocity components, so that the iteration convergence had been ceased.

Therefore, calculation of the eddy viscosity had been performed by means of a new algorithm that used a modification of the formula (2):

$$v_e = C_v \sqrt{k \varepsilon / \varepsilon}.$$  \hspace{1cm} (3)

Here $\varepsilon$ is a ratio of the turbulence-dissipation rate to the turbulence kinetic energy ($\varepsilon = \varepsilon / k$). Values of the parameter $\varepsilon$ have been defined by the solution of the differential equation [3] with supplementary items, which had not been accounted earlier.

Taking into consideration that relative errors of values are summarized at their multiplication and division, it is possible to demonstrate that calculation of the eddy viscosity by means of the formula (3) comes to be more precise. Since the ratio had changed in iterations much weaker than quantities $k$ and $\varepsilon$, inaccuracy of the calculated eddy viscosity reduced almost three times as compared with that produced by the formula (2). This helped to restore the iteration convergence and allowed to realize numerically the mathematical model of the heat and mass transfer in the glass furnace with returned gas flow.

According to a curve in Fig. 3, the eddy viscosity of the gas increases by many times at distance 1... 1.4 m from the air-inlet window in the front wall, owing to inhibition of the gas flow in a dead-end part of the furnace. Intensity of eddy mixing the fuel with air was essentially raised there, what had been resulted in an extremely short diffusion flame of fuel combustion. Its computer image is presented in Fig. 4.
Figure 3. Change of the eddy viscosity of the gases along the furnace

Figure 4. View from above on the diffusion flame in the glass furnace with returned gases flow

Combustion of natural gas in a short flame in entourage of the very hot air had produced extremely elevated temperature of the flame, reaching 2300...2500 °C at the front of burning. In the stagnant part of the gas space beyond the short flame, the temperature of gases had gone down, approaching gradually to the temperature of the molten-glass surface. As it is well known, a relatively low temperature level of the stagnant gas space allows zones of glass cooling to be organized at the end of the molten-glass basin of the glass furnaces with returned gas flow.

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