Mathematical Modeling of the Composition of the Combustion Products of the Heating Gas of a Coke Oven

Oleg U. Sidorov
NTI (branch) UrFU, Nizhny Tagil
o.iu.sidorov@urfu.ru

Natalija A. Aristova
NTI (branch) UrFU, Nizhny Tagil
natasha_17@yandex.ru

Abstract

In this work, the task is to construct a mathematical model and calculate with its help concentration and temperature fields, as well as the velocity distribution of gas sweats movement during the combustion of the heating gas in the vertical of the coke oven Structures of TDCs. Is being studied the effect of the excess air factor and the nature of the gas dynamic in the heating section of the coke oven to the concentration of the combustion products.

As a modeling area, two heating piers (vertical) were considered, located near the middle of the coke oven of the PVR system with a volume of 41.6 m3. We considered a three-dimensional problem with a partition of the modeling region along the x axis into 24 cells; along the y axis, by 13 cells; on the z axis, 24 cells. Vertical dimensions: along the axis x0.48 m; on the y axis, 0.40 m; on the z-axis - 7,2 m.

Simultaneous solution of three-dimensional equations of motion, heat energy transfer, mass transfer and kinetic interactions of gas flow components is carried out.

The methods of mathematical modeling are used to estimate the velocity fields, traces and temperatures in the heating section of the coke oven at an excess air factor in the range 1.2-1.6. The possibility of overheating of the upper part of the vertical due to the appearance of a turbulent vortex is shown. Extreme behavior of the nitrogen monoxide content is obtained depending on the excess air factor. It is shown that the presence of asymmetry of the boundary velocities at the inlet and outlet from the vertical leads to a decrease in the recirculation and an increase in the concentration of nitrogen monoxides in the flue gases.

Keywords: coke oven, kinetics, velocity, temperature, concentration field traces.

Introduction

Optimization of coke oven operating modes is actual task. Simulation of the combustion process of gaseous fuels will make it possible to trace the distribution of the temperature, concentration, velocity fields along the height of the combustion zone and after it. This will allow us to analyze the effect of gas dynamics and combustion on the heating of various zones Refractory masonry, the dependence of the composition of flue gases, especially such harmful constituents such as formaldehyde and nitrogen oxides, on the nature of motion of gas flows. To solve this type of problem it is necessary simultaneous consideration of gas-dynamic, concentration and thermal problems.

Formulation of the problem

The task is to construct a mathematical model and calculate with its help the concentration and temperature fields, and also distribution of speeds of movement of gas sweats at combustion of a heating gas in a vertical of coke oven of system PVR. The influence coefficient of excess air and the nature of gas dynamics in the heating space of the coke oven on the concentration of combustion products.

As the modeling area, two heating piers (vertical) were considered, located near the middle of the coke furnaces of the PVR system with a volume of 41.6 m3. We considered a three-dimensional problem with partitioning the modeling domain along the x-axis into 24 cells; on the y-axis - by 13 cells; on the z axis, 24 cells.

The vertical dimensions are chosen according to [1, 2]; overall dimensions: along the x0.48 m axis; on the y axis, 0.40 m; on the z-axis - 7,2 m.

Mathematical model

In solving the gasdynamic problem, the following equations were used [1]:

Movement

Here $b = u, v, w$ - are the velocity components; ρ - is the density.

Non-discontinuities

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0. \tag{2}$$

Integration of equations (1) was carried out within the framework of the method of finite differences using the "chess" grid [2,3]. The unknown pressure field was determined using the continuity equation (2) according to the procedure described [2,3]. The boundary conditions of the first kind were used to specify the velocity of the gas at the inlet and outlet from the vertical and the zero velocity values on the walls of the vertical.

The equations for the transfer of the concentrations of the components of the gas mixture in the form [1]

$$\frac{\partial(\rho C_i)}{\partial t} + \frac{\partial(\rho u C_i)}{\partial x} + \frac{\partial(\rho v C_i)}{\partial y} + \frac{\partial(\rho w C_i)}{\partial z} = \frac{\partial}{\partial x}\left(\frac{\mu}{Sc} \cdot \frac{\partial C_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\mu}{Sc} \cdot \frac{\partial C_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{\mu}{Sc} \cdot \frac{\partial C_i}{\partial z}\right) + S_i. \tag{3}$$

Here the designation of components

$i = O_2, N_2, CH_4, CO, CO_2, H_2, H_2O, CH_2O, NO$; S_i - the source terms of the $S_i = k_i \prod_m [C_m]^{n_m}$, where k_i - form rate constant; C_m - concentration of component m in mole fractions; n_m – the order of the chemical reaction by component m; Sc - the Schmidt number (it was chosen equal to 0.9 [1]).

When integrating Eq. (3), boundary conditions of the first kind were applied at the entrance to the vertical and on the laying of the vertical; At the exit from the vertical, we used boundary conditions of the third kind in the form

$$\frac{\partial C_i}{\partial z} = 0.$$

The heat energy transfer equation is chosen in the form [3]

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho u h)}{\partial x} + \frac{\partial(\rho v h)}{\partial y} + \frac{\partial(\rho w h)}{\partial z} = \frac{\partial}{\partial x}\left(\frac{\mu \cdot C_p}{\Pr} \cdot \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\mu \cdot C_p}{\Pr} \cdot \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{\mu \cdot C_p}{\Pr} \cdot \frac{\partial T}{\partial z}\right) + \frac{dQ}{dt} \tag{4}$$

Here μ, C_p, h, T - turbulent dynamic viscosity, heat capacity, enthalpy, temperature, respectively;

$\Pr$ - is the Prandtl number (it was chosen equal to 0.56 [1]);

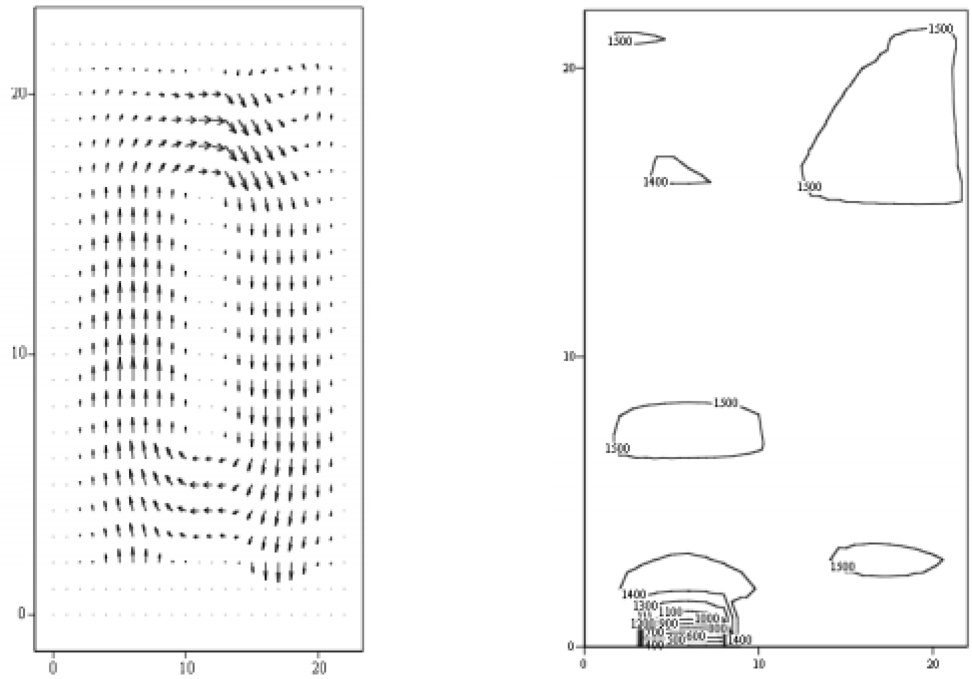
dQ/dt - the total rate of heat release from the reactions occurring during combustion of the gas mixture (see [4]).

When integrating equation (4), the boundary conditions were applied I-th kind on the basis of experimental values of temperature measurements in the conditions of Coke-chemical production of JSC "NTMK". The temperature of the gas flow at the entrance to the vertical is of the order of 1000 ° C, the temperature on the masonry about 12500C.

In modeling the combustion process, a coke oven gas was used as a fuel, the interaction of its components with air was carried out using model constructions detailed in [4].

Results

The results of the calculations in the vertical section (the middle along the y axis) heating partition with = 1, 2 are shown in Fig. 1 and 2. In this case, the same boundary conditions are set for the velocity at the input and output from the vertical (1 m / s). There is a fairly intensive recirculation movement of gas flows. There is a turbulent vortex in the upper right side of the vertical (Fig. 1 (a)). In the same place is the zone of elevated temperature (Figure 1 (b)), which can affect negatively for the life of refractories of this part of the masonry. Formation of nitrogen oxides and formaldehyde occurs throughout the vertical region (Figure 2 (a, b)).



(a) (b)

Fig. 1 Velocity (a) and temperature (b) fields

It is shown that the content of formaldehyde and carbon monoxide in flue gases decreases with an increase in the excess air factor. The content of nitrogen oxides passes through a maximum at about α = 1.4 - 1.45. This may be due to the onset with an increase in NO due to an increase in the N2 concentration in the input stream, and then to a decrease in the formation of NO, due to a decrease in the temperature in the vertical due to a decrease in the proportion of coke oven gas in the composition of the heating mixture.

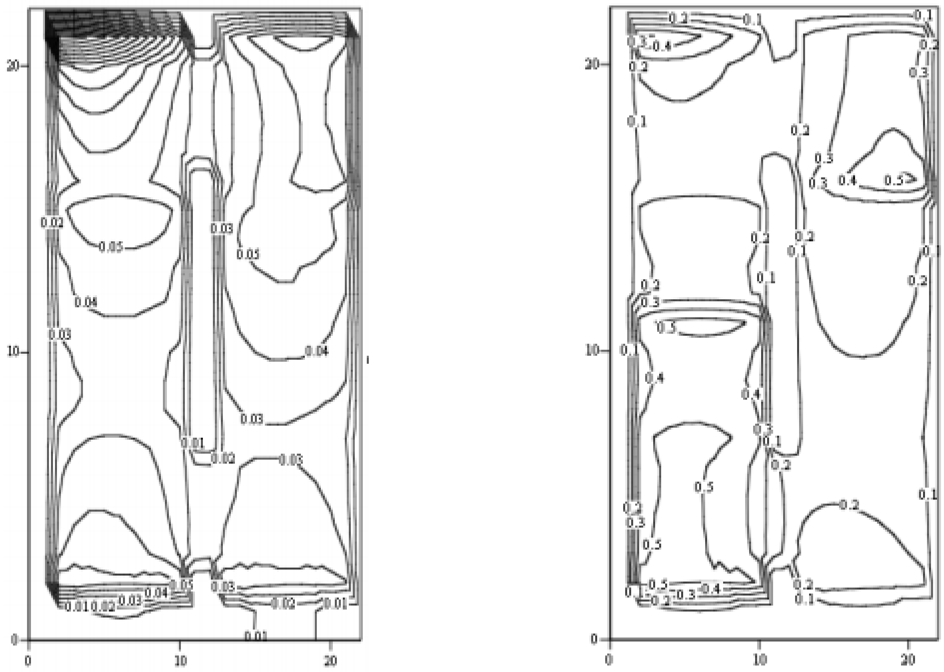


Fig. 2. Fields of CH_2O and NO concentration

Let us consider the regime of motion of gas flows with different boundary velocities at the inlet and outlet from the vertical. This can be due, for example, to their different temperatures. The results of calculations of the velocity field (□ = 1,6, the boundary velocity at the entrance to the vertical of 1 m / s) for two boundary values of the velocity at the exit from the vertical are given in Fig. 3. These data allow us to conclude that the asymmetry of the boundary velocities leads to a decrease and a complete absence of recirculation in the heating partition. This leads to an increase in the NO content of flue gases. An increase in the boundary velocity at the outlet from the heating partition from 1 to 1.98 m / s results in a practically linear increase in the concentration of nitrogen oxides by about 4%. The content of formaldehyde and carbon monoxide is reduced by approximately 35%.

Conclusions

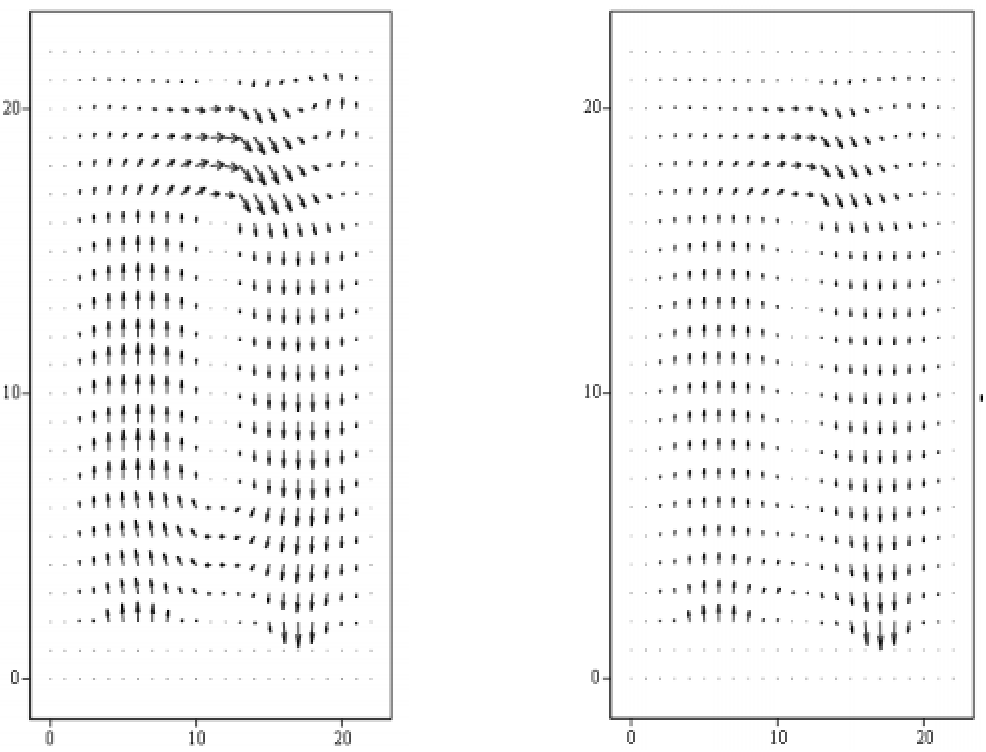
1. Methods of mathematical modeling have been used to estimate the velocity, concentration and temperature fields in the coke furnace heating section with an excess air factor in the range 1.2-1.6.

2. The possibility of overheating of the upper part of the vertical due to the appearance of a turbulent vortex is shown.

3. Extreme behavior of the content of nitrogen mono-oxides is obtained depending on the excess air factor.

4. It is shown that the presence of asymmetry of the boundary velocities at the inlet and outlet from the vertical leads to a decrease in the recirculation and an increase in the concentration of nitrogen monoxides in the flue gases.

The implementation of the model was carried out using the author's software package.



Limit velocity at 1,29 m/s vertical output   Limit velocity at 1,98 m/s vertical output

Fig. 3. Velocity fields for different limit velocities in the vertical output

References

1. Announcer P. A. Calculation and experimental study of the burner device for afterburning of the anode gas / P. A. Unannounced, A.A. Dekterev, A.A. Gavrilov, Yu.I. Storozhev // Thermophysics and Aeromechanics, 2007, Vol. 14, No. 1. C.151-160.

2. Sidorov O.Yu. Methods of finite elements and finite differences in electromechanics and electrotechnology. / O. Yu. Sidorov, F.N. Sarapulov, S.F. Sarapulov. - M.: Energoatomizdat, 2010. - 331 p.

3. Patankar S. Numerical methods for solving problems of heat transfer and fluid dynamics. / S. Patankar. - Moscow: Mir, 1984. - 152 p.

4. Sidorov O.Yu. Mathematical modeling of combustion of heating gas in the heating channel of a coke oven. / O.Yu. Sidorov, N.A. Aristova // Coke and Chemistry, № 8, 2017, C.23-29.