Eurasian ChemTech Journal 4 (2002) 147-151

The Modeling of Chemical Technological Process in the Fire Chambers

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Abstract

In this paper the results obtained by the method of numerical modeling of Ekibastuz coal burning in furnace on the example of fire chamber fixed on Aksy hydroelectric station are represented. Numerical experiment was carried out on the basis of three-dimensional equations of convective heat and mass transfer, taking into account the heat propagation, heat radiation, chemical reactions and multiphase structure of the medium. After the numerical experiment, the pictures of temperature distribution on the height of the chamber and concentration of CO, CO_2, ash and coke distribution along the chamber were obtained. The results are represented graphically.

Introduction

At the present time the investigation of combustion processes of solid fuel is of great interest due to the mounting ecological problems in many regions of Kazakhstan. Previously the main efforts were directed at the increase of efficiency of coal fuel use. However, presently, first of all, it is necessary to reduce to minimum or exclude completely the toxicantcy of combustion products [1].

Products of combustion contain different harmful substances and the emission of these components grows in to a great problem. Industrial development causes an increase in hydrocarbonaceous fuels' consumption. These fuels contain harmful and poisonous components such as carbonic oxide (CO), nitric oxide (NO), sulphur dioxide, acid sulphate, lead combinations and different hydrocarbons etc.

To decrease emissions of harmful substances various methods are applied, including special fire regimes (organization of combustion process), which suppresses the formation of harmful substances in flame and two-stage burning, when the burners work with low air surplus.

In this case numerical experiments became one of the most effective and suitable means for detail analysis and in-depth study of physical and chemical phenomena [2].

In contrast to construction of an operating reduced model of the chamber, the three-dimensional modeling with the application of modern computer technology enables to carry out deep analysis of all chamber's parameters and save time and finances. At the same time, without additional inputs, it is possible to obtain the full set of characteristics of a convective heat and mass transfer process in reactive media, intervene flexibly in the process at any stage and reproduce separate technical solutions (the configuration of the fire chamber and assembly and construction burners), to model the formation of harmful dust and gaseous emissions and to investigate the influence of previous preparation of coal on its ignition and combustion stabilization.

Mathematical model

Combustion of coal-dust flame is a very complex physico-chemical process for mathematical analysis. In the boilers, where coal-dust fuel burns down in the air stream, many interrelated processes occur. They are: complex aerodynamics, combustion under conditions of constantly changing temperature and component concentrations, heat exchange between the flame and the chamber surface. Simultaneous formation of carbon, nitrogen and sulphur oxide, corrosion hazardous and carcinogenic substances occurs.

A numerical experiment was carried out on the basis of three-dimensional equations of convective heat and mass transfer, taking into account the heat propagation, heat radiation, chemical reactions and the multiphase structure of the medium. To describe

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3-D motion of reacting flows in chambers, the following set of differential equations are used [3]:

Continuity equation:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x_i}(\rho u_i) \qquad (1)$$

Momentum conservation law:

$$\frac{\partial}{\partial t}(\rho u_i) = -\frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{\partial}{\partial x_j}(\tau_{i,j}) - \frac{\partial p}{\partial x_j} + \rho f_i \qquad (2)$$

Here f_i - volume forces; $\tau_{i,j}$ - strain tensor

Energy equation:

$$\frac{\partial}{\partial t}(\rho h) = -\frac{\partial}{\partial x_i}(\rho u_i h) - \frac{\partial q_i^{res}}{\partial x_j} + \frac{\partial p}{\partial t} + u_i \frac{\partial p}{\partial x_i} + \tau_{ij}\frac{\partial u_j}{\partial x_i} + s_q \qquad (3)$$

Here h – enthalpy; S_q - energy source.

Conservation law for substance components:

$$\frac{\partial}{\partial t}(\rho c_\beta) = -\frac{\partial}{\partial x_i}(\rho c_\beta u_i) - \frac{\partial j_i}{\partial x_i} + R_\beta \qquad (4)$$

where i=1, 2, 3; j=1, 2, 3; β=1, 2, 3.....N and R_β - source of matter

A standard *k-e* model of turbulency has been used to close off the system and model turbulent viscosity:

$$\frac{\partial}{\partial t}(\rho k) = -\frac{\partial}{\partial x_i}(\rho u_i k) + \frac{\partial}{\partial x_i}\left[\frac{\mu_{eff}}{\sigma_k}\frac{\partial k}{\partial x_i}\right] + \Pi - \rho\varepsilon \qquad (5)$$

$$\frac{\partial}{\partial t}(\rho\varepsilon) = -\frac{\partial}{\partial x_i}(\rho u_i \varepsilon) + \frac{\partial}{\partial x_i}\left[\frac{\mu_{eff}}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_i}\right] + c_{\varepsilon 1}\frac{\varepsilon}{k}\Pi - c_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} \qquad (6)$$

where $$\Pi = \left[\mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\rho k\delta_{i,j}\right]\frac{\partial u_i}{\partial x_j} \qquad (7)$$

Also the model correlation for turbulent viscosity was used:

$$\mu_t = c_\mu \rho k^2/\varepsilon \qquad (8)$$

Point concentration of solid matter was determined by means of balance equations for monodispersion solid matter with the avarage particle diameter. To determine the mixture concentration the homogeneous model was used. Velocities of solid particles were equaled local gas velocity. For turbulent viscosity taking into acount solid particle the next relation was used:

$$\mu_{P,eff} = \mu_{G,eff}\left(1 + \frac{\rho_P}{\rho_G}\right)^{-\frac{1}{2}}$$

Each of the equations was written for average values of parameters.

Equation (2)-(6) may presented in the following generalized form:

$$\frac{\partial}{\partial t}(\rho\Phi) = -\frac{\partial}{\partial x_i}(\rho u_i \Phi) + \frac{\partial}{\partial x_i}\left(\Gamma_{\phi,eff}\frac{\partial \Phi}{\partial \rangle_i}\right) + S_\phi \qquad (9)$$

Here Φ is the generalized transfer variable. By means of Φ we may denote velocities components u, v, w, temperature T (or enthalpy $h = c_pT$), components concentration c, k, ε, Γ_Φ – generalized exchange coefficient, S_Φ - source term in transfer equations.

Calculation of turbulent flows with chemical reactions is based on the knowledge of chemical kinetics and methods of modeling of turbulent transfer processes. To determine the source term in equation (4) which is connected with chemical reaction rate, it is necessary to model correctly kinetics of chemical reactions. These reactions take place between fuel and oxidant in combustion space of the boiler. Local distribution of reacting components and temperature significantly influence on the reaction rates. The amount of energy, emitted in chemical reactions, the flame temperature and the nature of combustion products are very important characteristics in estimation of solid substances influence. Using the solid particles as fuel is most probable.

The model of coal dust combustion which is being used in this paper takes into account an integral oxidizing reaction of fuel components down to a stable final products of reaction. Intermediate reactions and the formation of intermediate products haven't been taken into consideration. The model of integral reaction was used based on according to the fact that many chemical reactions proceed several stages. The slowest reaction determines the rate of the whole reaction.

Reaction rate may be represented in the form:

$$\omega_\beta = \frac{dc_{AB}}{dt} = k(T)c_A c_B \qquad (10)$$

The reaction rate depends on the temperature and concentration of reacting components *A* and *B* (initial, intermediate and final products). The constant of reaction rate *k(T)* may be written in the form of Arrenius law [4], as the exponential temperature dependence:

$$k(T) = k_0 e^{-E/RT} \qquad (11)$$

Here k_0 is the constant, which doesn't depend on the temperature in the first approach, *E* [kkal/mol] is the activation energy, *R*=1.986 [kkal/mol grad] is the gas constant. The values of kinetic constants are determined in the experiment.

Simplified models are being used in this paper. These models take into account only chemical reactions of key components since the detail modeling of all passing reactions is possible only in the simple cases, because of large computational costs. For example, in the case of carbon oxide burning. Information about reactions and their kinetic data have been taken from [5].

Equation (9) is complex and it doesn't have analytical solution. This system can be solved only numerically. At the present time the problem-oriented software for the many tasks of continuum mechanics is available.

In this paper software package FLOREAN for 3-D modeling of coal-dust combustion in furnaces of boilers was used. This program enables to calculate velocity components *u*, *v*, *w*, temperature *T*, pressure *P*, concentration of combustion products and other characteristics of combustion process all over the combustion space and at its exit. Pressure is determined through the connection between the continuity equation and the equation of motion by means of Patankar's Simple-method [6].

For numerical solution of (9) the calculation region is divided by the differences net into discrete points or volumes. Derivatives are expressed by approximate expressions through the differences in function values in net vertices.

The optimum method to solve this task is the method of control volume. To present differential equations (9) in finite-difference form, equations (9) are integrated over the control volume:

$$\iiint_V \frac{\partial}{\partial t}\rho\phi_n dV = \iint_A \left(-(\rho\phi_n u_i) + \partial_{\text{TM}} \frac{\partial \phi_n}{\partial x_i} \right) \cdot \vec{n} dA_{no} + \iiint_V S_{\phi_n} dV \qquad (12)$$

Using the mean value theorem we can write approximate value each of integrals in (12). We will obtain algebraic equation for every control volume and every unknown variable Φ_p. Coefficients of equation are functions of Φ_p variable and they are connected with values in other equations. The obtained system is solved by sweep method.

Since system (9) doesn't have any analytical solution, then in order to determine calculation error, experimental data may be used. Experimental data are obtained at the acting power stations.

Results of the numerical experiment

Fig. 1 shows distribution of maximum, minimum and average temperature along the chamber height in crossections (X,Y). The experimental data are represented here too. Curve minimums are connected with low temperature of fuel mixture (150°C) supplied in the chamber space through the burners.

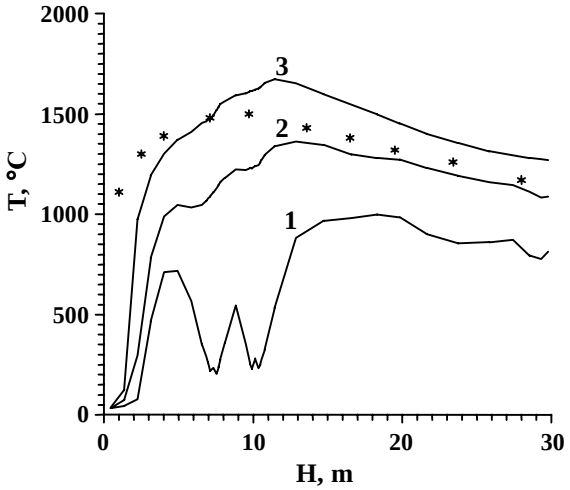

Fig. 1. Temperature distribution to chamber height: 1 – minimum value, 2 – average value, 3 – maximum value; line – calculation, ∗ - experiment.

Significant differences of calculated and experimental values of temperature are seen in the region of ignition and extinction. It apparently may be explained by assuming that the coal was burned completely. Endothermal restoration of carbonic acid gas in the coke is neglected, though this fact leads to temperature increase. Simultaneously, there is an increase in the outlet of flying components with an increase in temperature.

Figures 2-6 show the picture of fuel burning down with the curves of oxygen, carbonic acid gas CO_2 and carbon oxide CO, ash and cokes concentration change.

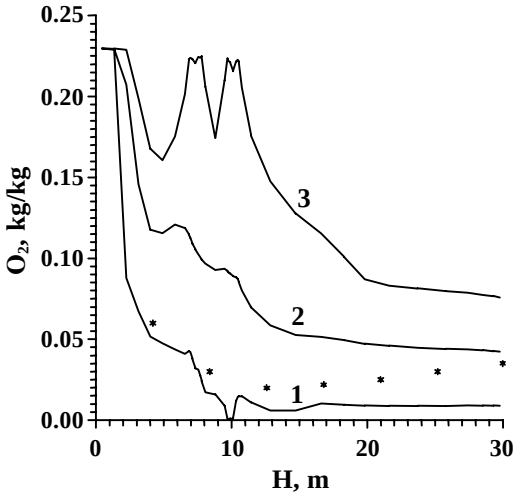

Fig. 2. O_2 concentration distribution along the chamber: 1 – minimum value, 2 – average value, 3 – maximum value; line – calculation, ∗ - experiment.

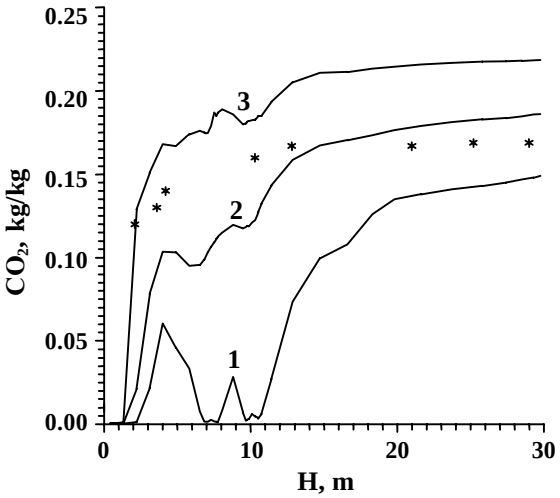

Fig. 3. CO_2 concentration distribution along the chamber: 1 – minimum value, 2 – average value, 3 – maximum value; line – calculation, ∗ - experiment.

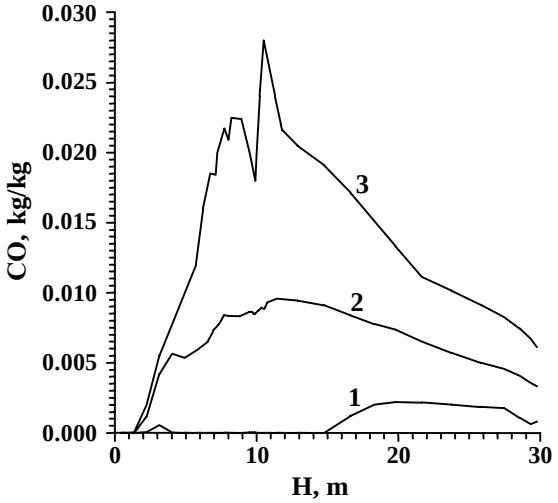

Fig. 4. CO concentration distribution along the chamber: 1 – minimum value, 2 – average value, 3 – maximum value.

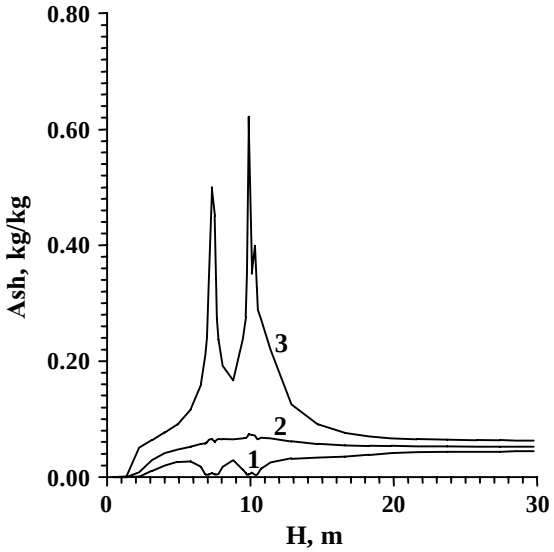

Fig. 5. Ash concentration distribution along the chamber: 1 – minimum value, 2 – average value, 3 – maximum value.

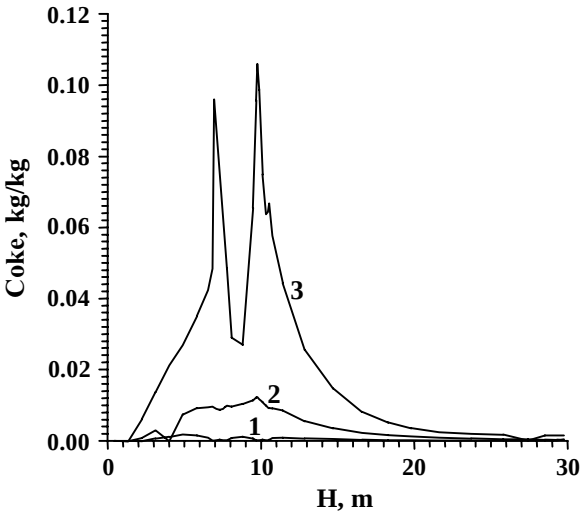

Fig. 6. Coke concentration distribution along the chamber: 1 – minimum value, 2 – average value, 3 – maximum value.

Observed also is the base formation of gases in the torch which takes at the level of burners.

The maximum difference of calculation and experiment are seen in the region of ignition and extinction of flying matters. The main reason for this is that there is a determination of the gas burning rate by one stage model of piroliz where the set of kinetic constants for all the entire temperature range are used in contrast to a two stage model of piroliz when these constants have various values for every temperature. The figures show that the regions with maximum difference coincide with regions having high concentrations of carbon oxide (Fig.4).

An analysis of figures 2 – 6 shows that the rate of burning down decreased up to the point of chamber. Taking into account the model of this work experimental profiles correspond to boundary conditions at the chamber outlet.

At the exit of the chamber CO_2, CO and ash concentration is 16%, 0,5% and 10% respectively, which is agreeable to standard values. The distribution character of all concentrations, listed in this paper is modeled sufficiently and it agrees with the published experimental data.

Conclusions

According to the results of modeling a conclusion may be made that favorable conditions are created in the chamber with the opposite position of vertical burners when the torch is strongly twisted, provided a stable torch ignition and intensive combustion of coal dust,. Agreement with the experimental data shows the reliability of the chosen model. Obtained results enable to create new technologies of burning using high-ash and damp solid fuel. Application of the results may help to increase efficiency of a combustion process and to optimize the process of high-ash coal dust fuel burning with the goal of decreasing pollutant emissions.

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Received 18 September 2001.