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MATHEMATICAL MODELING OF GASIFICATION AND COMBUSTION OF COAL-WATER FUEL IN A CYCLONE FURNACE EXTENSION

The article provides a method of mathematical modeling using the software package "SigmaFlow", which allows to describe processes of aerodynamics and heat transfer in the thermal processing of fuels. The features of combustion and gasification of coal-water fuel were considered in the simulation and also kinetic constants and activation energies that describe most fully real process of fuel reprocessing were used. As a result of modeling processes of gasification and combustion of coal-water fuel in a cyclone furnace extension with a horizontal axis cylindrical chambers, temperature fields and concentration fields of coal particles in the cross section of furnace extension were obtained. Also the product compositions of thermal processing were defined.

Keywords: coal-water fuel, software package "SigmaFlow", thermal processing, cyclone furnace extension, temperature field, substance concentration

Introduction

Ukraine has significant reserves of low caloric coal, broad and effective application of which will greatly expand the power base of the country. Production of coal-water fuel on the basis of low caloric coals is promising for their application and can be used in various energy units [1]. Since the coal-water fuel is a relatively new type of fuel, and its mechanism of thermal processing is different from the processing of coal, then for the effective use of coal-water fuel in the energy it is necessary to study the operating parameters and the basic regularities of thermal processing of coal-water fuel with the development of new designs of combustion units.

Modern combustion units are very diverse in aerodynamic configurations and aerodynamics is one of the factors determining the processes of combustion and heat transfer in combustion devices. Mathematical modeling based on physical laws describing the aerodynamics and heat transfer processes is widely used in the design and construction of combustion units. One of the software packages that effectively describes the processes of aerodynamics and heat transfer in combustion devices is a package for numerical simulation "SigmaFlow" (Krasnoyarsk branch of the Institute of Thermophysics. SS Kutateladze SB RAS, Russia), which showed high accuracy in the study of a wide class of hydrodynamic and thermal processes and optimization of the aggregates of objects of power, hydropower and nuclear power [2-4].

Statement of problem and research objectives

Thermal processing of coal-water fuel proposed to be performed in the cyclone furnace extension with a horizontal axis cylindrical chambers. Cyclone furnace extension consists of a pre-treatment chamber, where leaking and burning of volatiles of coal-water fuel take place, and the chamber for combustion or gasification. This furnace extension has a tangential aerodynamic configuration of coolant flow. An autothermal swirling flow technology, that provides high-intensity and high degree of carbon conversion process, is supposed to use in the furnace extension [5].

The objective of this work is to research the furnace processes of gasification and combustion of coal-water fuel in a cyclone furnace extension by means of mathematical modeling in the software package "SigmaFlow" considering the distinctive features of thermal processing of coal-water fuel.

Research methods and data analysis

When modeling with "SigmaFlow" software package it is assumed that gases flow is spatial and turbulent. It is believed that turbulent flow, as well as laminar, can be described by the Navier-Stokes equation. In the program "SigmaFlow" the standard k-ε model is used as the turbulence model, which allows to describe a sufficiently wide class of turbulent flows, including both shear and gravitational turbulence, and represents the turbulence model of the first level of closure. The equations describing this model are as follows:

$$\frac{\partial \rho \mathrm{k}}{\partial t} + \nabla(\rho \mathrm{v} \cdot \mathrm{k}) = \nabla\left(\left(\mu + \frac{\mu_t}{\sigma_\mathrm{k}}\right) \cdot \nabla \mathrm{k}\right) + P - \rho\varepsilon, \quad (1)$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla(\rho \mathrm{v} \cdot \varepsilon) = \nabla\left(\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right) \cdot \nabla \varepsilon\right) + \mathrm{C}_1 \frac{\varepsilon}{\mathrm{k}} P - \mathrm{C}_2 \rho \frac{\varepsilon^2}{\mathrm{k}}, \quad (2)$$

where k – kinetic energy of the turbulent fluctuations; ε – rate of dissipation of turbulence; v – time averaged velocity field; μ_t – turbulent viscosity; μ – dynamic (molecular) viscosity; P – rate of generation of turbulence; $\nabla \mathrm{k}$, $\nabla \varepsilon$, C1, C2 – constants of the standard model, which, according to [6] make: $\nabla \mathrm{k}$=1,0, $\nabla \varepsilon$=1,3, C1=1,44, C2=1,92.

Energy conservation equation is considered in the following form:

$$\frac{\partial \rho h}{\partial t} + \nabla(\rho \mathrm{v} h) = \nabla(\lambda \nabla T) + S_h, \quad (3)$$

where h – enthalpy of multicomponent medium; λ – thermal conductivity; S_h – the source term responsible for inflow (outflow) of energy in the chemical reaction, radiation, or other processes.

Coal-water fuel properties such as thermal conductivity, density, specific heat capacity, enthalpy, dynamic viscosity, molecular mass are defined by mass fractions of its components.

The transfer equation of concentration of components is as follows:

$$\frac{\partial \rho Y_m}{\partial t} + \nabla(\rho \mathrm{v} Y_m) = \nabla(\rho D_m \nabla Y_m) + S_{Ym} \quad m = 1 \ldots N, \tag{4}$$

where Y_m – the mass fraction of the m component; D_m – diffusion coefficient of the m component; S_{Ym} – source term responsible for the change in the components of the chemical reaction processes or any other processes.

Turbulent flow near the wall has a complex structure with significant gradients. In the inner area, which occupies about 20% of the thickness of the boundary layer, about 80% of the turbulent energy is generated. For modeling of the near-wall flows wall functions method is used, connecting the flow parameters with the distance to the wall, which is an analytical solution of simplified solutions of turbulent flow. Simplification core is based on the following assumptions: the local equilibrium of energy of turbulent fluctuations (local turbulence production rate is balanced by rate of viscous dissipation), the constancy of the shear stress along the layer, a negligible pressure gradient along the flow, the local isotropy of dissipating vortices, universality of the velocity profile (weak dependence on the Reynolds number).

To solve the equation of energy transfer, widely known method of control volume is used. The essence of this method consists of dividing the computational domain into control volumes (Fig. 1) and the integration of the initial conservation equations for each control volume to obtain the finite-difference relations. Properties of the method are described in detail in the literature [7, 8]. In the given package multi-block structured curvilinear grids with excludable areas are used.

Heat exchange process is a complex radiation-convective interaction between the furnace environment and the bounding surfaces in significantly nonisothermal conditions, complex aerodynamics and fuel combustion, multiple reflection and scattering of selective radiation. Higher temperature level of environment and surfaces causes the predominance of radiative heat transfer. Therefore, during the thermal calculation, increased requirements to accounting for radiation component in the total heat transfer are presented.

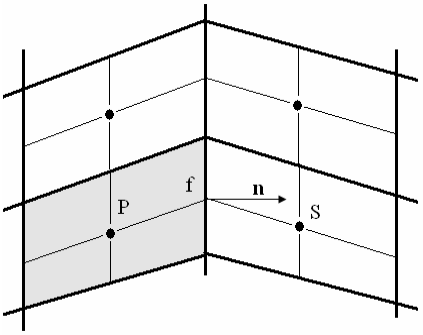


Figure 1 - On the computation of flow through the face of control volume

In this paper to describe the motion of the fuel particles the Lagrangian method is used. In the simulation of particle motion major forces acting on the particle are interfacial force (aerodynamic resistance force) and gravity.

The equation of motion of the particle is written as:

$$\frac{dU_{ip}}{dt} = C_w A_p \frac{\rho}{2} U_r (U_i - U_{ip}) - \rho g_i, \quad (5)$$

where

$$C_w = \frac{24}{Re_p} f_k, Re_p = \frac{U_r d_p \rho}{\mu_{mol}}, U_r = \left(\sum_{i=1}^{3} (U_i - U_{ip})^2\right)^{1/2},$$

d_p – diameter of the particle; U_i – i-th component of the the gas velocity; $U_i = \overline{U}_i - U_i'$, U_i – average i-th component of the gas velocity; U_i' – pulsating component of the gas velocity; U_{ip} – i-th component of the particle velocity; C_w – coefficient of resistance.

Coefficient f_k for different Re_p values, can be written as follows:

$$f_k = \begin{cases} 1, Re_p \ll 1 \\ 1 + 0{,}15 Re_p^{0{,}687}, Re_p \leq 1000 \\ 0{,}44 \left(\frac{Re_p}{24}\right), Re_p > 1000 \end{cases} \quad (6)$$

Accounting for the effect of turbulence on the motion of the particles is made by introducing random fluctuations of the gas velocity in the equation of motion for the particles.

It is assumed that the coal-water fuel is represented by a discrete set of particles, which are fed through the nozzles into the combustion chamber. For the simulation of combustion and gasification of coal-water fuel in the "SigmaFlow" program a modified diffusion-kinetic model, represented in the form of successive stages, is used.

The first stage consists in heating and evaporation of moisture from the fuel. During evaporation of moisture a single drop evaporation model is used. This model is

calculated basing on the value of the amount of water vapor on the particle surface and in the bulk:

$$N_i = k_C(C_{i,s} - C_{i,\infty}), \quad (7)$$

where N_i – molar vapor flow; k_C – mass transfer coefficient; $C_{i,s}$ – vapor concentration on the particle surface; $C_{i,\infty}$ – vapor concentration in the bulk.

After evaporation of moisture occurs particle decay. Particles, formed after the collapse, burn by model of coal particles ignition and combustion [9,10]. To describe the processes of gasification of coal-water fuel in the mathematical model reactions of steam-coal conversion were implemented. However, it is necessary to consider that the process of burning of coal-water fuel differs from coal combustion [11,12] and thus values of the kinetic constants and activation energies differ. In the study of combustion and gasification of coal-water fuel in the proposed software package additional reaction and more accurate values of the equilibrium constants and activation energies for the said fuel [13-15] are laid. This allowed to describe the processes of combustion and gasification of coal-water fuel most fully and approximated to the real conditions.

Reduction of weight and diameter of the coal particle occurs in the process of burning, the density of the particle remains constant.

Changes in particle diameter due to the combustion are described by equation:

$$\frac{d\delta}{d\tau} = \frac{2}{\rho_к} K_s^c, \quad (8)$$

where $\rho_к$ – density of the coke residue; K_s^c – carbon-burning rate.

Particle temperature is determined by the equation of energy conservation:

$$\frac{m_ч C_ч}{4\pi r_ч^2}\frac{dT}{dt} = \varepsilon\sigma\left(T_{рад}^4 - T_ч^4\right) + \alpha_{конв}(T_г - T_ч) + \frac{QH}{4\pi r_ч^2}, \quad (9)$$

where $C_ч$ – heat capacity of the particle; ε – degree of blackness of the particle; σ – coefficient of blackbody radiation; $T_{рад}$ – temperature of the radiating volume; $T_ч$ – temperature of the particle; $\alpha_{конв}$ – coefficient of convective heat transfer; Q – specific thermal effect of reaction.

Weakening of convective heat transfer, which is explained by the release of vaporous and gaseous substances from the surface of coal particles in coal-water fuel during their heating, can be taken into account by using the Nusselt number as a function of Peclet number of external washing (Pe) and Peclet number of gas ($\overline{Pe}$):

$$Nu = 2 + \frac{Pe}{2} - \frac{37}{960}Pe^2 - \frac{Pe\overline{Pe}}{4} - \frac{\overline{Pe}}{2}, \quad (10)$$

where $$\overline{Pe} = \frac{w\delta}{a}, \quad (11)$$

where w – release rate of the reaction products and volatile.

Since heat exchange with the gas atmosphere is more intensive during carbon particles combustion [16], the coefficient, considering the effect of the combustion process on the convective heat transfer, is introduced in mathematical model.

$$\alpha_{конв}^{гор} = \alpha_{конв} K_{гор}, \quad (12)$$

where $\alpha_{конв}^{гор}$ – effective coefficient of convective heat transfer between the burning coal particles and gas; $\alpha_{конв}$ – the coefficient of convective heat transfer from the particle surface in the absence of combustion.

It is known [17] that the coefficient $K_{гор}$, considering the influence of the combustion process on the convective heat transfer between the particles of coal dust and gas environment, in a specified range, depends little on the particle size and the oxygen concentration in the gas environment. In the temperature range of 1200-1600 K coefficient $K_{гор}$ can be written as follows:

$$K^{гор} = 145 e^{-\frac{5000}{T_г}}. \quad (13)$$

The software package "SigmaFlow" allows to get the temperature and concentration of gaseous components and coal particles in the central section and the length of each chamber as well as the velocity vector field for each chamber of burner device.

When modeling the processes of thermal processing of coal-water fuel it was assumed that air temperature at the inlet of each chamber is 400 °C and the fuel temperature is 150 °C. Heating of energy carriers at the inlet of furnace extension is performed to achieve the required temperature level of processes of thermal processing [18]. Calculations were made applied to coal-water fuel made Ukrainian gas coal with combustion heat of 15,1 MJ/kg and a solids content of 61,5%.

Computational grid is imposed on the investigated object (cyclone furnace extension) after the calculations. Grid model of the cyclone furnace extension is shown in Fig. 2.

When modeling it is assumed that flow rate of oxidant and process temperature were taken as basic control parameters to achieve the required composition of the products of thermal processing of the fuel. Characteristics of temperature fields in the cross section of the cyclone furnace extension are shown in Fig. 3.

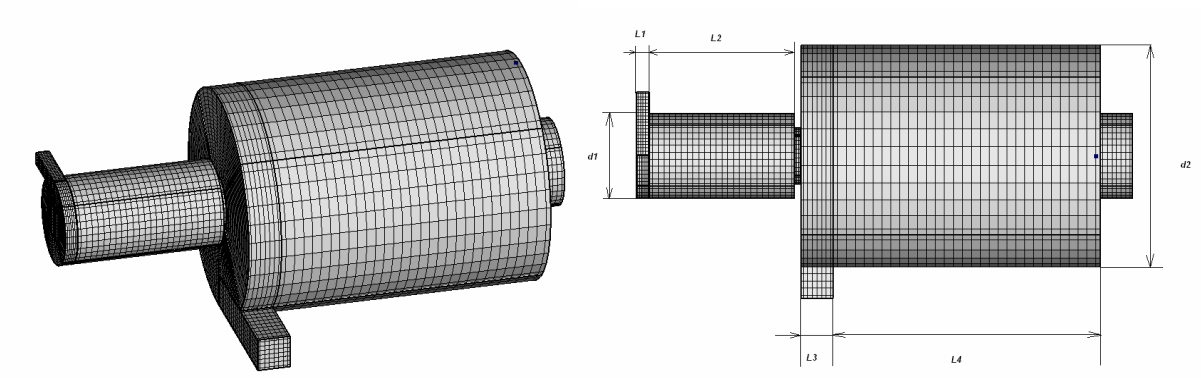
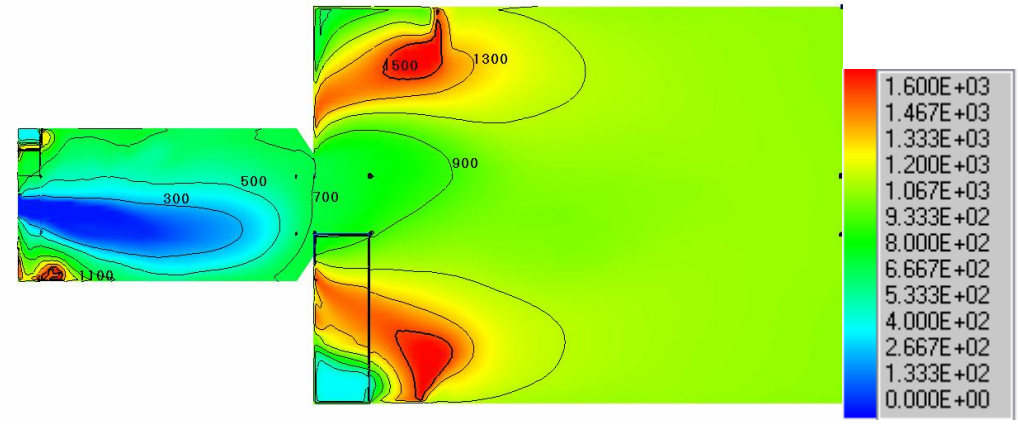


Figure 2 – Grid model of cyclone furnace extension

a



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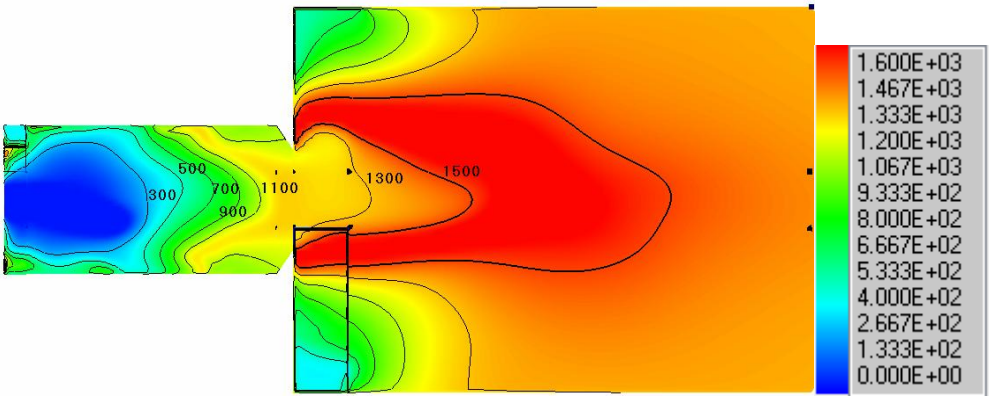

Figure 3 – The temperature field in the central cross section during the gasification (a) and combustion (b) of coal-water fuel, °C

As can be seen from the received data, during the gasification of coal-water fuel, the temperature in the first furnace extension chamber is 300-500 °C, which is sufficient to release and partial combustion of volatiles of the fuel. In the second furnace extension chamber, where the afterburning of volatile and fuel gasification occur, the temperature level is about 900 °C.

During combustion of coal-water fuel in the first furnace extension chamber release and burning of volatiles occur. Temperature in this case is 900-1100 °C. In the second chamber there is an active burning of coke residue of the fuel and the temperature is 1300-1500 °C. It is important that the flow of combustion products of coal-water fuel over the cross section of the cyclone furnace extension has a uniform temperature at the outlet.

The concentration of coal particles in the cross section of the cyclone furnace extension during the gasification and combustion of coal-water fuel is shown in Fig. 4.

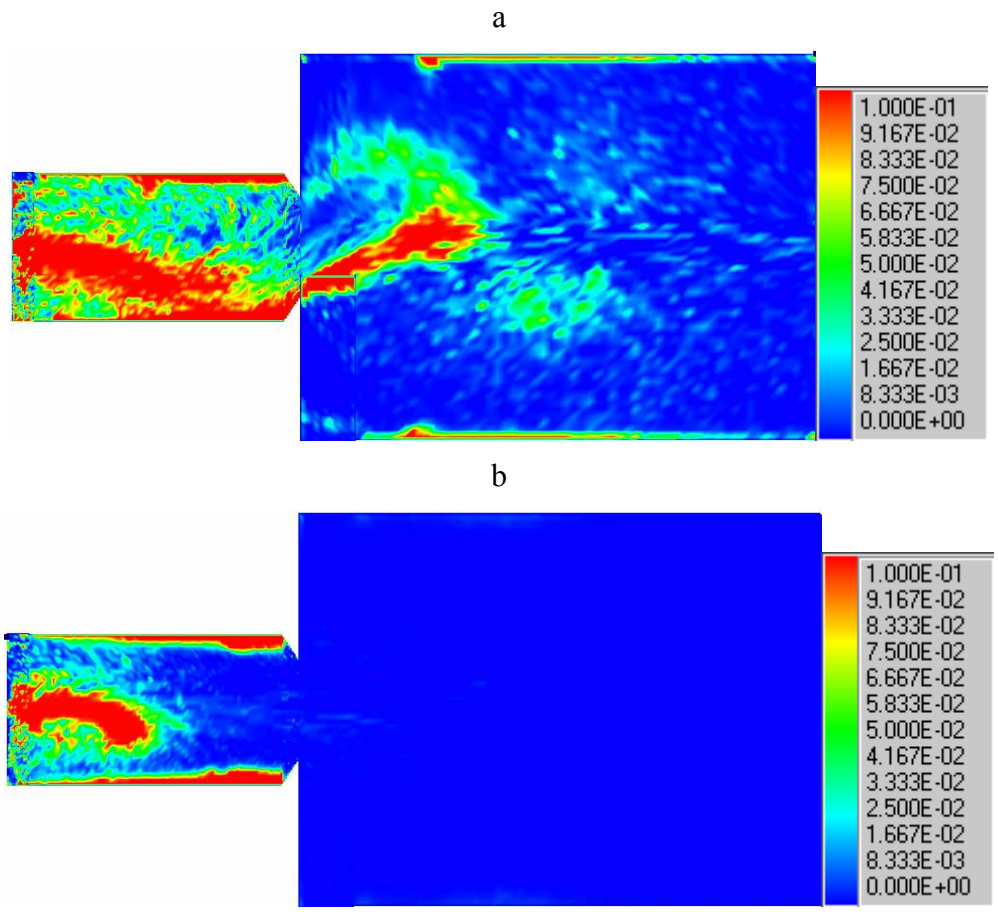

Figure 4 - The concentration of coal particles in the central cross section of the furnace extension during the gasification (a) and combustion (b) of coal-water fuel, kg/m^3

Presented results show that there is little mechanical incomplete combustion of fuel during the thermal processing of coal-water fuel in a cyclone furnace extension. The degree of conversion of the carbon from during the gasification of coal-water fuel is 90,8% and during combustion it reaches 93,3%. These indicators are significantly higher than during the thermal processing of coal dust (83-87%).

Composition of products of thermal processing at the cyclone furnace extension outlet obtained by modeling are shown in Table 1.

Table 1

Composition of the products of thermal processing of coal-water fuel

The composition of the products of combustion, % vol.	Gasification	Combustion
CO	14,1	~ 0
H_2	5,9	~ 0
CO_2	8,5	11,8
H_2O	16	16,5
CH_4	6,8	~ 0
N_2	48,7	66,2
O_2	~ 0	5,5

Gas containing 26,8% of the combustible components is produced during gasification of coal-water fuel in a cyclone furnace extension, while calorific value of gas is 4,9 MJ/m^3. During the gasification of fuel it is possible to maintain such oxidant consumption, which sets the appropriate value for reducing and oxidizing gas components, determined by the technology of its usage.

During combustion coal-water fuel in a cyclone furnace extension, the composition of the combustion products indicates the occurrence of complete combustion reaction with the formation of CO_2 and H_2O end-products.

The obtained results of mathematical modeling of thermal processing of coal-water fuel in a two-chamber cyclone furnace extension describe the processes occurring in combustion devices of this type, and can be used to create furnace extensions for coal-water fuel processing.

Conclusions

Analyzing the results obtained, it can be concluded that the use of the software package "SigmaFlow" considering features of coal-water fuel combustion processes allows to investigate the thermal processing of coal-water fuel in a sufficiently wide range.

Thermal processing of coal-water fuel is encouraged to implement in double chamber cyclone furnace extension with a horizontal axis of cylindrical chambers using autothermal technology in a twisted thread.

Established that the thermal processing of coal-water fuel in a cyclone furnace extension is expedient to carry out at air heating up to 400 °C and fuel heating up to 150 °C. It provides the necessary temperature level of gasification processes (900-1000 °C) and combustion processes (1300-1500 °C). The degree of conversion of the carbon during the gasification of coal-water fuel is 90,8%, during the combustion it reaches 93,3%.

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