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ANALYSIS AND WAYS FOR ADVANCING OF MATHEMATICAL MODEL OF PULVERIZED COAL IGNITION AND COMBUSTION

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Abstract. An analysis of mathematical models of ignition and burning of a single particle and a coal cloud is given. Models which take into account the presence of ash in particles, the influence of the ratio of the amount of coal and primary air (excess coefficient) and the size of coal particles on the ignition process are presented and analyzed. It is shown that simplifications in mathematical models in most cases lead to a loss of accuracy and therefore the results cannot be used for practical purposes. Simulation of complex air supply processes by approximation of uniformity also leads to questionable results. A significant influence on the ignition and combustion of coal particles affects the content and intensity of the release of volatile substances and the chemical reactions that occur in this case. The rate of volatiles yield is proposed to be calculated according to the Arrhenius law, and the activation energy and frequency factor are considered to be those that do not depend on the type of coal, but are determined only by the temperature of the particle. Taking into account heat transfer by radiation and a decrease in the particle diameter during combustion has a positive effect on the results obtained. According to the results, the reactivity and losses with underburning significantly depend on the initial diameter of coal particles. Most models do not take into account the change in temperature inside the particles during heating, ignition and combustion in the apparatus, but there are works that are specifically devoted to the study of temperature fields inside the particles and the influence of the particle shape on the combustion rate. Modeling showed that motion relative to the gas leads to an intensification of heat transfer between the particles and the environment, while the volatile matter yield time decreases at a high ambient gas temperature. A decrease in the rate of combustion chemical reactions is noted with an increase in the concentration of water vapor in the gaseous medium around the particle, i.e. oxygen diffusion is the limiting factor in particle combustion. The most complete and physically correct gas dynamics during combustion is calculated in models where known turbulence models are used, such as the standard k-ε model, RNG k-ε model, BSL model and SST model. At the end of the article, the concepts for improving the model of ignition and combustion of coal particles are outlined.

Keywords: pulverized coal, combustion, devolatilization, particle, chemical reaction, ignition.

1. Introduction

Pulverized coal combustion is widely used in energy sector since late 19th century. This fact caused pioneer experimental and theoretical studies of the ignition and combustion processes for the single coal particle as well as multiple coal particles. Pilot studies of a single coal particle combustion were conducted by Nusselt with assumption of isothermic process as well as combustion rate exceptionally depends on oxygen diffusion. He has made calculation of the burnout time.

In similar studies of Gumz and Orning calculations were made with an assumption about zero oxygen concentration at the surface of the coal particles.

Further studies of Predvoditelev in addition to oxygen diffusion chemical reaction rates at the surface of the coal particles were taken into account.

Vulis made an assumption of the constant oxygen concentration in environment and calculated burnout time of the coal particle with the application of the convective theory for the carbon combustion. Also he made an attempt to determine ash influence on the combustion rate.

Kantorovich tried to take into consideration chemical reactions that take part inside coal particles as well as variable mass flow of the particles, diffusion ant isothermic conditions for study of the coal particle combustion.

Baskakov, Reznyakov, Pomerantsev, Shagalova and Arefyev for the first time took into account polydispersity of the coal particles by replacing them with equivalent monodispersed coal particles. It was thought that small particles as well as volatile matter burnout instantly and this process is isothermic along the flame length.

Despite incorrect physical assumptions in pioneer studies devoted to the mathematical modeling of the coal combustion their results had a great significance for the pulverized coal combustion theory development and served as fundamentals for the development of pioneer techniques for the burner furnaces calculation.

2. Methods

The creation and rapid development of electronic computing machines, the Internet, electronic means of storing, transmitting, reproducing and analyzing information caused revolutionary changes in exact and technical sciences.

The enormous speed of computing machines and the development of information technologies have opened wide opportunities for the development and application of new theories and mathematical methods of research in all branches of science. The fundamental difference from the previous situation is that complex technical problems can be solved in an exact formulation that is inaccessible to analytical methods of solution.

The approach to evaluating a particular computational method has changed significantly. The most universal method, which allows a simple implementation on machines, turns out to be valuable. On the contrary, a method based on the particular features of the problem or the engineer ability is now of little use. Many computational methods, which led to cumbersome counting and were previously considered impractical in manual counting, have now turned out to be quite working. At the same time, purely analytical constructions leading to inconvenient computational algorithms have lost their former importance. Iterative, difference, variational, probabilistic and similar methods for solving problems, which have convenient calculation algorithms, are universal and can be applied to a wide range of problems, are widely used.

The means of searching and analyzing the received scientific information have radically changed. Now almost all the results of scientific research, issued in the form of publications, are posted on the Internet. The availability of most of the information on the Internet allows instantly get all the results of research wherever there is Internet coverage. Thanks to the Internet and the developed effective search systems, among which the most common is Google, each researcher has access to almost all publications on the chosen topic, including the problem of burning solid fuels.

3. Results and discussion

Among the pioneer studies devoted to the mathematical modeling of the coal particle combustion in a quiescent environment where in addition to conductive heat transfer and chemical reactions kinetics radiative heat transfer was taken into account could be mentioned investigation of Takahashi [1].

This made possible more precisely define coal to primary air ratio, coal particles

size and ash content influence on the ignition process of the coal particle as well as influence of the combustion chemical reactions rate on the unburned carbon content.

Temperature rises of coal particle and surrounding air are given by the following equations:

$$\frac{\pi \cdot c_p^{/} \cdot d_p^3}{6} \cdot \frac{dT_p}{d\tau} = \pi \cdot d_p^2 \cdot \left(q_r + q_c - q_p\right), \tag{1}$$

$$\frac{\pi \cdot c_a^{/} \cdot d_p^3}{6} \cdot \frac{dT_a}{d\tau} = \pi \cdot d_p^2 \cdot q_p, \tag{2}$$

where $c_p^{/}$ – specific heat of the coal particle, J/(m^3·K); d_p – diameter of the coal particle, m; T_p – temperature of the coal particle, K; q_r – heat radiated from the flame and surface of the boiler furnace to the coal particle, W/m^2; q_c – heat caused by chemical reactions between carbon and oxygen on the surface of the particle, W/m^2; q_p – heat transferred from the particle to the surrounding air, W/m^2; $c_a^{/}$ – specific heat of the air J/(m^3·K); T_a – air temperature, K; τ – time, s.

It is shown that the ignition times of some pulverized coals of 60, 50 and 5 microns in size are respectively about 34–44, 28–36 and 27–34 milli-seconds.

Neglecting of chemical reactions kinetics that take place within gas flow and chemical content change of the gas flow (certainly, this causes to the complication of calculation process) reduce the results value with regard to the practical application in comparison with real conditions of the pulverized coal combustion.

R.K. Ahluwalia and P.M. Chung [2] assuming one-dimensional combustion process, continuity and quiescence of the surrounding air, analytically studied an influence of the coal particle initial temperature, surrounding air pressure, particles size and air temperature on the ignition time.

It was assumed in the mathematical model that at the surface of the coal particle single step exothermic chemical reactions of the Arrhenius type commence. Heat transfer between coal particle and surrounding air takes place due to the heat conduction (air velocity is equal to zero) and radiation, however, specific heat flux at the surface of the coal particle is a constant.

Solving the equations that describe coal particle ignition process was provided analytically using asymptotic ignition theory and Laplace transformation technique.

Governing partial differential equations are reduced to an integral equation containing a double integral.

In turn, integral equation is further simplified to an ordinary differential equation for its integration.

For a typical case, on reducing the particle radius from 100 microns to 5 micron at a combustion temperature of 6250 °C, ignition time dropped from 19 milli-seconds to 0.25 milli-seconds. On the other hand, ignition time for a particle of 55 microns radi-

us jumped from 10 milli-seconds to 25 milli-seconds when the combustor temperature is changed from 6250 °C to 3750 °C.

Also, it has been found that the ignition time slightly depends on the combustor pressure.

Shortcomings in the model are due to the assumptions that do not match to the real combustion process that take place within thermal units.

Thus, the results of the study are predominantly of theoretical nature and could be applied in thermal engineering with some limitations.

Smith та Smoot [3] tried to make up mathematical model of the coal particle combustion in the reactor taking into account chemical reactions kinetic for coupled one-dimensional gas dynamic and heat transfer equations solving.

It was proposed comprehensive approach for the solving of the one-dimensional mathematical model of the coal particle combustion.

In particular, model takes into account moisture evaporation from the coal particle, devolatilization and heterogeneous char oxidation.

System of ordinary differential equations was integrated by means of numerical technique.

Some relationships of gas chemical constituents (nitrogen, carbon monoxide and dioxide), coal and ash constituents from the reactor length are obtained and further were compared to the experimental data.

Taking into consideration primary and secondary air inlet technique into reactor physical justification of the one-dimensional equations is quite doubtful as well as chemical reactions of devolatilization and coal particle combustion are too simplified.

In the study [4] critical size of the coal particle at the moment of its ignition and extinction was defined by means of numerical technique.

The mathematical model takes into account mass reduction of the coal particle in the combustion process. It was mentioned that coal particles of a size below 350 microns may not undergo gas-phase ignition.

Paper [5] is devoted to the experimental and theoretical investigation of the coal particle ignition within the temperature range of 1300–2000 K. It was experimentally determined approximately 70 % of carbon burns out within 30 milli-seconds; devolatilization rates increased with increasing oxygen concentration; temperature, energy from the oxidizing volatiles appears to be fed back to the coal particles, increasing their temperature; particle size inhomogeneity plays an important role in determining the overall devolatilization rate; particle luminosity was apparent in less than 5 milliseconds.

A flame sheet mathematical model consists of the equations as follows.

The radius of the flame sheet is given by:

$$r_{sh} = G_v \cdot \frac{\left(\nu_{pr} - \nu_{O_2}\right)}{4 \cdot \pi \cdot c_a \cdot D_{O_2} \cdot ln\left(1 + \frac{\left(\nu_{pr} - \nu_{O_2}\right) \cdot \chi_{O_2}}{\nu_{O_2}}\right)}. \quad (3)$$

The energy balance for the flame sheet is expressed as:

$$G_v \cdot H = \frac{G_v \cdot c_{mp\,v} \cdot \left(T_{sh} - T_p\right)}{1 - e^{\frac{-G_v \cdot c_{mp\,v}}{4 \cdot \pi \cdot \lambda_{pr}} \cdot \left(\frac{r_{sh} - r_p}{r_{sh} \cdot r_p}\right)}} + \frac{G_v \cdot \left(\nu_{pr} \cdot c_{mp\,pr} - \nu_{O_2} \cdot c_{mp\,O_2}\right) \cdot \left(T_{sh} - T_a\right)}{1 - e^{\frac{G_v \cdot \left(\nu_{pr} \cdot c_{mp\,pr} - \nu_{O_2} \cdot c_{mp\,O_2}\right)}{4 \cdot \pi \cdot r_{sh} \cdot \lambda_{pr}}}} +$$
$$+ 4 \cdot \pi \cdot r_p^2 \cdot \sigma_0 \cdot \varepsilon_{sh} \cdot \left(T_{sh}^4 - T_p^4\right) + \tag{4}$$
$$+ 4 \cdot \pi \cdot r_{sh}^2 \cdot \sigma_0 \cdot \varepsilon_{sh} \cdot \left(T_{sh}^4 - T_w^4\right) \cdot \left[1 + \left(1 - \varepsilon_{sh}\right) \cdot \left(1 - \frac{r_p}{r_{sh}}\right)\right].$$

The unsteady energy equation for the devolatilizing coal particle is given by:

$$m_p \cdot c_{m\,p} \cdot \frac{dT_p}{d\tau} = \frac{G_v \cdot c_{mp\,v} \cdot \left(T_{sh} - T_p\right) \cdot e^{\frac{-G_v \cdot c_{mp\,v}}{4 \cdot \pi \cdot \lambda_{pr}} \cdot \left(\frac{r_{sh} - r_p}{r_{sh} \cdot r_p}\right)}}{1 - e^{\frac{-G_v \cdot c_{mp\,v}}{4 \cdot \pi \cdot \lambda_{pr}} \cdot \left(\frac{r_{sh} - r_p}{r_{sh} \cdot r_p}\right)}} + \tag{5}$$
$$+ 4 \cdot \pi \cdot r_p^2 \cdot \sigma_0 \cdot \left[\left(1 - \varepsilon_{sh}\right) \cdot T_w^4 + \varepsilon_{sh} \cdot T_{sh}^4 - T_p^4\right],$$

where r_{sh} – radius of the flame sheet, m; G_v – volatile mass loss rate, kg/s; ν_{pr} – kmoles of product generated per kg of volatiles on the flame sheet or particle surface, kmol/kg; ν_{O_2} – kmoles of oxygen required per kg of volatiles released for the combustion products assumed on the flame sheet or particle surface, kmol/kg; c_a – mole concentration of the air, kmol/m^3; D_{O_2} – effective diffusivity of oxygen, m^2/s; χ_{O_2} – ambient mole fraction of oxygen; H – heat of reaction per mass of volatile, J/kg; $c_{mp\,v}$ – heat capacity of the volatiles, J/(kg·K); T_{sh} – flame sheet temperature, K; λ_{pr} – thermal conductivity of the gas, W/(m·K); r_p – radius of the particle, m; $c_{mp\,pr}$ – heat capacity of the products, J/(kmol·K); $c_{mp\,O_2}$ – heat capacity of oxygen, J/(kmol·K); σ_0 – Stefan-Boltzmann constant, W/(m^2·K^4); ε_{sh} – flame sheet emissivity; T_w – flow tube wall temperature, K; m_p – mass of the particle, kg; $c_{m\,p}$ – heat capacity of the particle, J/(kg·K).

In [6] mathematical model of the coal particle combustion with detailed description of the radiative heat transfer is proposed.

Main features of the model are similar to those ones in a flame sheet model for single droplet of a liquid fuel, but mathematical model [6] takes into account concentric luminous mantle around the coal particle that created by volatiles as well as radiative heat transfer between coal particles.

The mathematical model consists of the equations as follows.

Energy balance equation:

$$\frac{1}{r^2}\cdot\frac{d}{dr}\left[r^2\cdot\left(\lambda_p\cdot\frac{dT_p}{dr}-q_r\right)-\rho_p\cdot v_r\cdot r^2\cdot c_{mp}\cdot T_p\right]+q^{/}=0, \quad (6)$$

where λ_p – thermal conductivity of the coal particle, W/(m·K); v_r – radial velocity, m/s; ρ_p – density of the coal particle, kg/m^3; $q^{/}$ – volumetric heat source, W/m^3.

The boundary conditions are: for $r=r_1$ $T=T_1$ and $q_r=q_1$; for $r=r_2$ $T=T_2$ and $q_r=q_2$. Indexes "1" and "2" refer to two different coal particles, accordingly.

Thus, within this model, luminous mantle created by volatiles is considered as a heat transfer medium (conduction and radiation) between coal particles and flame.

The results of the experimental and numerical modeling allow to determine that the most of the sooty constituents are oxidized at the flame boundary and volatiles form a jetlike tail that flows appears to be completely random with respect to the flow direction.

Despite detailed description of the radiative heat transfer mathematical model does not take into account a significant contribution, for example, from convective heat transfer between coal particle and surrounding gas as well as transient nature of the devolatilization process. It is also not clear how homogeneous and inhomogeneous chemical reactions of the coal combustion are taken into account.

The results obtained by Musarra, Fletcher, Niksa and Dwyer [7] disproved validity of the flame sheet model. They made up a model of heat and mass transfer processes in vicinity of the single coal particle entrained in a laminar air flow. Two-dimensional mathematical models of the devolatilization and coal particle combustion in the boundary layer between particle surface and the bulk air flow are proposed.

Authors claim that within the range of the coal particle size of 20–200 microns and low Reynolds number Stokes two-phase flow occurs, where coal particle velocity value is close enough to that one for surrounding medium.

Time-dependent equations of conservation of momentum, energy, and chemical species for the gas phase are used for mathematical modeling.

Light and heavy volatiles are represented by methane and benzene.

Devolatilization process is described by the chemical reactions as follows:

$$CH_4+1{,}5O_2\rightarrow CO+2H_2O, \quad (7)$$

$$C_6H_6+4{,}5O_2\rightarrow 6CO+3H_2O, \quad (8)$$

$$CO+0{,}5O_2\rightarrow CO_2, \quad (9)$$

$$CO_2\rightarrow CO+0{,}5O_2. \quad (10)$$

The coal can be oxidized heterogeneously by both oxygen and carbon dioxide to yield carbon monoxide:

$$C + 0{,}5O_2 \rightarrow CO, \tag{11}$$

$$C + CO_2 \rightarrow 2CO. \tag{12}$$

Particle properties are treated as time-dependent but spatially uniform.

Simulations indicate that flame sheet approximations are not applicable during devolatilization. Parametric studies indicate that particle heating is dominated by homogeneous volatiles combustion for large particles and by heterogeneous reaction for small particles.

Shortcomings of the model are as follows: constant density value of the gas-phase medium around the coal particle, element contents of the coal does not counts hydrogen, ash, sulfur as well as chemical reactions of carbon with water are absent.

Discrepancy between experimental and numerical data is quite admissible only for temperature range of 1500–2200 °C.

In study [8] the results of experimental investigation and mathematical model of devolatilization for large pressed coal particles (3–9 mm) are shown.

It was assumed that the overall rate of coal devolatilization is expressed by an Arrhenius formula, in turn, activation energy, E, and the equivalent frequency factor, A, are independent of coal type, and depend only on the final temperature of the coal particles.

Experimental investigation of the rate of devolatilization was conducted by exposing coal particles to an inert gas (argon) flow for the temperature range of 1173–1733 K.

Since permanent temperature measurement of the coal particle during its heating is a very difficult task the results of the study are carried out as dependences of the parameters from the final temperature of the coal particle. Thus, averaged values of the mass loss of the coal particles were determined that was stipulated by devolatilization in the temperature range from the initial one at the beginning of the heating to the final temperature.

The experimental results were necessary for constants determining in mathematical model.

The kinetics equation of devolatilization of coal particles is:

$$\frac{dm_v}{d\tau} = \left(m_{v\,f} - m_v\right) \cdot A \cdot e^{\frac{-E}{R \cdot T_p}}, \tag{13}$$

where m_v – mass fraction of volatiles; $m_{v\,f}$ – final value of mass fraction of volatiles; A – frequency factor of coal devolatilization, s^{-1}; E – activation energy of coal devolatilization, J/mol; R – general gas constant, J/(mol·K).

The energy equation with devolatilization of a large spherical particle is as follows:

$$\rho_p \cdot c_{m\,p} \cdot \frac{\partial T_p}{\partial \tau} = \overline{\lambda}_p \cdot \left(\frac{\partial^2 T_p}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial T_p}{\partial r} \right), \tag{14}$$

where $\overline{\lambda}_p$ – average conductivity of coal particles during coal particle devolatilization, W/(m·K).

Boundary conditions:

$$\left. \frac{\partial T_p}{\partial r} \right|_{r=0} = 0, \tag{15}$$

$$\left. \overline{\lambda}_p \cdot \frac{\partial T_p}{\partial r} \right|_{r=r_f} = \alpha \cdot \left(T_{ps} - T_{pf} \right) + \varepsilon_{ps} \cdot \sigma_0 \cdot F_r \cdot \left(T_{ps}^4 - T_{p0}^4 \right), \tag{16}$$

where α – convective heat transfer coefficient, W/(m^2·K); T_{ps} – surface temperature of coal particles, K; T_{pf} – final value of the surface temperature of coal particles, K; ε_{ps} – emissivity of the surface of the coal particle; F_r – angle coefficient; T_{p0} – initial temperature of the coal particle, K.

Initial conditions:

$$T_p(\tau, r)\big|_{\tau=0} = T_{p0}. \tag{17}$$

This is a versatile mathematical model, since activation energy of coal devolatilization and frequency factor of coal devolatilization depend on the coal particle final temperature only and do not depend on the coal type.

The only parameter determined from experimental data and necessary for devolatilization modeling is m_{vf} which depends on coal type.

In mathematical model of devolatilization [9] equations of heat and mass transfer are coupled with those ones for kinetics of pyrolysis.

In particular, study [9] is dedicated to the coal particle size influence as well as pressure and temperature of the medium where devolatilization occurs on the processes of the heat and mass transfer and kinetics of the chemical reactions.

Figure 1 shows a simplified technique of the coal particle combustion described in [10]. A mathematical model describes combustion processes at the surface of the particle at surrounding gas medium.

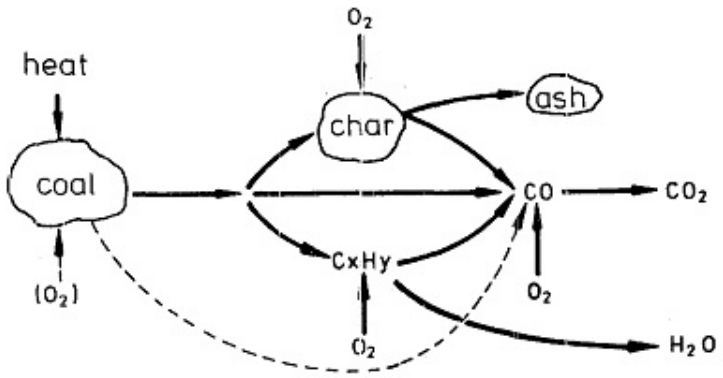
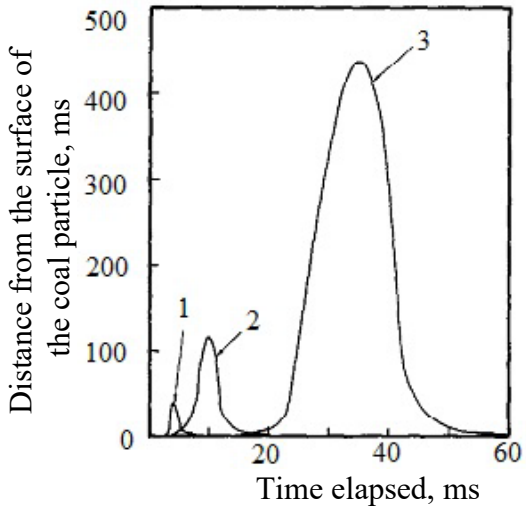


Figure 1 – Coal particle combustion model

In study [11] experimental facilities were used to determine temperature of the coal particle as well as surrounding gas in a combustion process. The results of the investigations are shown in figure 2.



1 – d_p=20 mkm, 2 – d_p=40 mkm, 3 – d_p=100 mkm

Figure 2 – Expansion of flame zone away from particle surface

The model calculations predicted that the particle temperature was more than 400 °C higher than the surrounding gas temperature.

In study [12] percolation model for coal char particle combustion and fragmentation is developed. Applying this model porosity increment and oxygen effective diffusivity within the char particle could be calculated.

Assuming an initially uniform porosity of the char particle, a critical porosity is calculated (0.84) at which the particle surface layer breaks into fragments. The fragmentation porosity upon particle reactivity and burnout times are evaluated.

The char fragments which separate from the particle upon the surface layer reaching critical porosity will be of the low reactivity type, e.g., inertinites (since the reactive components will be consumed preferentially), and that their probability of burnout in the tail end of the flame will be low despite their small size. These fragments will therefore likely contribute to the unburned carbon losses due to increased carbon

carry over into the stack.

Among major shortcomings of the model insufficient validation could be outlined since its verification was confirmed for certain coal types.

In study [13] mathematical model of the irregularly-shaped carbon char particle is proposed.

The conservation equations used to follow the mass, velocity and temperature of a particle as it burns in the laminar flow reactor are as follows:

$$v_p \cdot \frac{dm_p}{dx} = -R_s \cdot \pi \cdot d_p^2, \tag{18}$$

$$m_p \cdot v_p \cdot \frac{dv_p}{dx} = -m \cdot g - 3 \cdot \pi \cdot \mu_a \cdot d_p \cdot \left(v_p - v_a\right), \tag{19}$$

$$\frac{m_p \cdot v_p \cdot c_{m\,p}}{\pi \cdot d_p^2} \cdot \frac{dT_p}{dx} + \frac{2 \cdot \lambda_p \left(T_p - T_a\right)}{d_p} \cdot \frac{B}{e^B - 1} + \sigma_0 \cdot \varepsilon_p \cdot \left(T_p^4 - T_w^4\right) = R_s \cdot H, \tag{20}$$

where R_s – overall burning rate on external surface area basis, kg/(m^2·s); μ_a – gas viscosity, Pa·s; g – gravitational constant, m/s^2; B – convective (Stefan-flow) energy parameter that is determined as follows:

$$B = -\frac{\left(1 - \nu_{O_2}\right) \cdot R_s \cdot d_p \cdot c_{mp\,a}}{2 \cdot M_c \cdot \lambda_p}, \tag{21}$$

where ν_{O_2} – oxygen stoichiometric coefficient; $c_{mp\,a}$ – gas heat capacity, J/(kg·K); M_c – molecular weight of carbon.

The overall burning rate of the particle is described by:

$$R_s = k_c \cdot \left(\chi_{O_2} \cdot c_{pr}\right)^n, \tag{22}$$

where k_c – chemical rate coefficient, kg/(m^2·s); c_{pr} – total gas concentration; n – oxygen reaction order.

In turn, chemical rate coefficient is calculated from equation:

$$k_c = A \cdot e^{\frac{-E}{R \cdot T_p}}. \tag{23}$$

The external diffusion rate coefficient is given by:

$$k_d = \frac{2 \cdot M_c \cdot D_{O_2}}{\left(1 - \nu_{O_2}\right) \cdot d_p}. \quad (24)$$

The effective heat released per gram of carbon consumed is calculated from the heat of combustion of the two reactions:

$$H = \left(1 - \psi\right) \cdot H_{CO} + \psi \cdot H_{CO_2}, \quad (25)$$

where ψ -an energy parameter defined as the moles of CO_2 formed per mole of carbon reacted (equals to 0.35).

Chemical reactions of the coal particle combustion:

$$C + 0{,}5O_2 \rightarrow CO, \quad (26)$$

$$C + O_2 \rightarrow CO_2. \quad (27)$$

An orientation-dependent, shape-correction factor is defined as:

$$S_p = \frac{d_p}{l_{max}}, \quad (28)$$

where $l_{\max}$ – particle diameter measured by the sizing slits, m.

Mathematical model is one-dimensional, therefore it does not take into account an actual element contents of coal (contents of hydrogen, sulfur, moisture and ash) that leads to the omission of the influence of the homogeneous and heterogeneous chemical reactions on the combustion process.

In study [14] analysis of the ignition process of the single coal particle and clouds of particles as well as flame propagation is conducted. Variation of temperature difference between particle surface and center with time for a reactive particle is shown (fig. 3) as well as temperature of coal particle surface during combustion that were obtained experimentally.

Figure 3 shows that the surface temperature exceeds that of the center as the ignition point is approached. At or close to the point of ignition, however, the temperature gradient through the particle changes sign with the center heating faster than the surface. The detailed implication of this is that, if the particle ignites heterogeneously before it pyrolyzes then, when it does so, quite possibly it will pyrolyze from the inside out rather than from the outside in.

Figure 4 shows an initial drop in gas temperature as the relatively colder volatiles leave coal particle but with a gradient reversal after about 1 s, indicating the initiation or presence of reactions at that point.

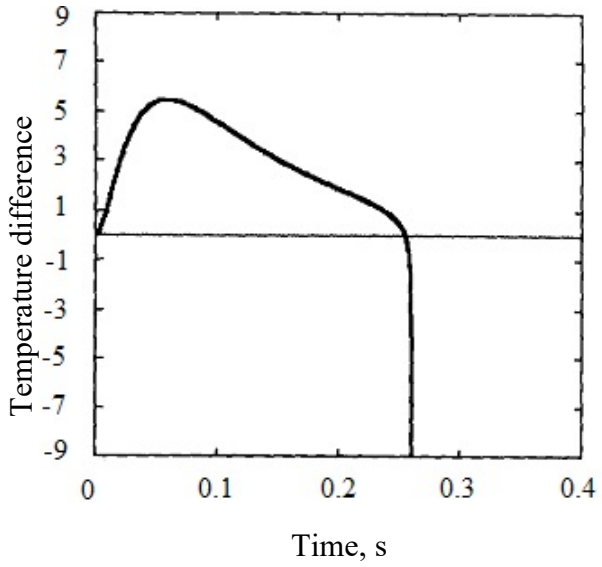
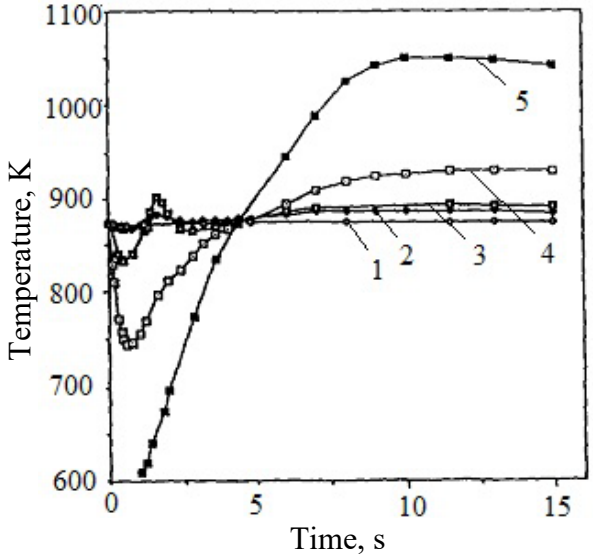


Figure 3 – Variation of temperature difference between particle surface and center with time for a reactive particle



1 – 2.5 mm from surface; 2 – 2.0 mm; 3 – 1.5 mm; 4 – 1 mm; 5 – particle surface

Figure 4 – Temperature of the coal particle surface during combustion

Figure 4 also shows that all points have about the same temperature at about 4.5 s. The results clearly show that combustion after ignition is at a location remote from the surface.

Authors stated that extension of that largely single-particle work to large dispersions is now required for credibility of such research in relation to engineering practice.

In study [15] authors stated that char particles in the 50–500 microns size range, 50–600 Hz frequencies and 100–150 K temperature excursions were observed when the particle temperature was about 2270 K.

Frequency of oscillations is calculated by:

$$f = \frac{4 \cdot 10^{-3} \cdot T_{pr}}{r_p \cdot \delta_{bl}}, \tag{29}$$

where δ_{bl} – boundary layer diameter around the particle, m.

For the particle burnout time approximation is used as follows:

$$\tau = 80 \cdot r_p^2. \tag{30}$$

Figure 5 shows oscillation frequencies as a function of coal particle diameter.

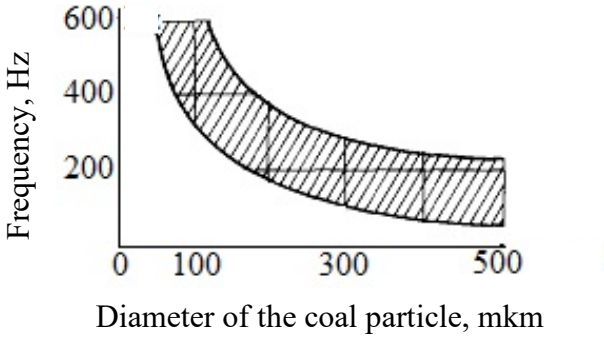


Figure 5 – Oscillation frequencies as a function of coal particle diameter

Study [16] is devoted to the attempt of development of the mathematical model for the group ignition of a cloud of coal particle.

Some assumptions were made within the mathematical model: cloud of coal particle is a spherical body located in a quiescent surroundings, coal particle is a spherical body as well and considered as a point sourced of heat and mass, during devolatilization heterogeneous chemical reactions at the surface of the coal particle occur, radiative heat transfer between coal particle and the walls of the thermal device is neglected.

The results of calculations testify that ignition is heterogeneous if the cloud is dilute and homogeneous if the cloud is dense under the same ambient conditions, a minimum ignition time for a given set of initial conditions corresponding to a certain cloud denseness; ignition time is less sensitive to the denseness of the cloud at higher ambient temperatures.

Despite quite good comparison of experimental and numerical these comparisons should be approached with caution since the experimental conditions and geometries may be vastly different than those used in the numerical study.

In study [17] a theoretical study is carried out of the combustion of nonspherical carbonaceous particles in the regime of shrinking core reaction.

The calculations show the particle shape to become increasingly nonspherical with the progress of combustion and this change to be more pronounced for particles with larger initial aspect ratios. For particles of equal initial volume, the burnout time

decreases slightly with the initial aspect ratio. For example a particle of initial aspect ratio 3.2 requires 12 % less time to reach 80 % burnout compared to a spherical particle of the same initial volume.

In paper [18] the effect of coal particle agglomeration during pulverized coal combustion is studied using a plug-flow model of a practical coal combustor.

Burnout time of the coal particle that accounts its agglomeration is given by the expression:

$$\tau_{coag} = \frac{\rho_p \cdot R_\mu \cdot (T_a + T_w) \cdot d_p^2}{32 \cdot M_c \cdot D_{O_2} \cdot P_a}, \tag{31}$$

where R_μ – ideal gas constant, J/(mol·K); P_a – air pressure, Pa.

The results of this work indicate that, in agreement with general observations, agglomeration will have little impact on pulverized coal combustion in typical combustors.

In work [19] experimental studies have shown that both char particle diameter and apparent density vary as burning progresses in combustion environments typical of pulverized coal combustors. In this paper, the intrinsic kinetics-based char oxidation model is described, and a particle population balance model for pulverized coal char combustion is presented.

Diffusion coefficient is proposed to substitute by Knudsen diffusion coefficient that can be expressed as:

$$D_{Kn} = \frac{1715 \cdot r_{por} \cdot \varphi_p \cdot \sqrt{T_p}}{S_p}, \tag{32}$$

where r_{por} – pore radius, m; φ_p – coal particle porosity.

The mean pore radius:

$$r_{por} = r_{por\,0} \cdot \frac{\varphi_p \cdot (1-\varphi_p) \cdot \overline{\rho}_{p0} \cdot \overline{F}_{ch0}}{\varphi_{p\,0} \cdot (1-\varphi_{p\,0}) \cdot \overline{\rho}_p \cdot \overline{F}_{ch}}, \tag{33}$$

where $r_{por\,0}$ – pore radius at the onset of char oxidation, m; $\overline{\rho}_p$ – apparent density of ash-free particle at the onset of char oxidation, kg/m^3; $\overline{F}_{ch}$ – specific surface area of the char particle, m^2/kg; $\varphi_{p\,0}$ – particle porosity at the onset of char oxidation; $\overline{\rho}_{p\,0}$ – apparent density of ash-free particle at the onset of char oxidation, kg/m^3; $\overline{F}_{ch\,0}$ – specific surface area at the onset of char oxidation, m^2/kg.

Assuming steady-state burning, gas and particle temperatures satisfy the following particle energy balance equation:

$$\frac{M_c \cdot D_{O_2\ bl} \cdot Sh \cdot P_a}{R_a \cdot T_a \cdot d_p \cdot \psi_{O_2} \cdot {}_{\Delta}\overline{V}} \cdot ln\left(\frac{1-{}_{\Delta}\overline{V} \cdot \frac{P_{O_2\ par}}{P_a}}{1-{}_{\Delta}\overline{V} \cdot \frac{P_{O_2}}{P_a}}\right) \cdot H = -\frac{Nu \cdot \lambda_p}{d_p} \cdot \frac{k}{1-e^k} \cdot \left(T_P - T_a\right) + \\ + \varepsilon_p \sigma_0 \cdot \left(T_p^4 - T_w^4\right), \quad (34)$$

where $D_{O_2\ bl}$ – oxygen bulk diffusion coefficient in boundary layer surrounding the particle, m^2/s; ${}_{\Delta}\overline{V}$ – change in volume upon reaction per unit oxygen consumed, m^3/mol; $P_{O_2\ par}$ – oxygen partial pressure in ambient gas, Pa; ψ_{O_2} – moles of oxygen reacted per mole carbon gasified; Nu – Nusselt number; k – coefficient that is calculated by:

$$k = \frac{{}_{\Delta}\overline{V} \cdot d_p \cdot c_{mp\ a}}{M_c \cdot \lambda_p \cdot Nu} \cdot \frac{M_c \cdot D_{O_2\ bl} \cdot Sh \cdot P_a}{R_a \cdot T_a \cdot d_p \cdot \nu_{O_2} \cdot {}_{\Delta}\overline{V}} \cdot ln\left(\frac{1-{}_{\Delta}\overline{V} \cdot \frac{P_{O_2\ par}}{P_a}}{1-{}_{\Delta}\overline{V} \cdot \frac{P_{O_2}}{P_a}}\right). \quad (35)$$

The model is shown to predict many characteristics experimentally observed during the combustion of pulverized coal chars, including variations in the mode of burning and reductions in char reactivity owing to thermal annealing while burning. Calculations indicate that char particles formed during devolatilization that have relatively high apparent densities contribute significantly to unburned carbon in ash.

In study [20] a mathematical model that consists of coupled equations of gas dynamics, heat transfer and coal particle combustion is proposed. The behavior of the air-coal mixture using the Navier-Stokes equations for gas and particle phases, accompanied by a turbulence model. The undergoing chemical reactions are described by the Arrhenian kinetics. Heat transfer via conduction and radiation is considered.

Among major shortcomings of the model a simplified approach to the coal particle combustion could be outlined since it was described by single chemical reaction with empirical constants. The mathematical model does not take into account non-spherical shape of the coal particles, ash content, intrinsic kinetics as well as sulfur oxides formation.

In work [21] the burning rate, surface temperature, drag, and extinction conditions of a single char particle moving in a gas are computed numerically.

A simple model of heterogeneous reactions (11), (12) and the gas-phase reaction (9) is applied. A mathematical model of the coal particle motion in the gas phase consists of continuity equations, momentum balance for laminar flow, equation of state for ideal gas, equation of energy conservation as well as mass concentration for constituents (oxygen, carbon oxide and carbon dioxide). Heat capacity for gas is consid-

ered to be constant.

When there is an infinitely thin diffusion flame in the gas around the particle, equation of energy conservation as well as mass concentration for constituents can be conveniently replaced by transport equations for the Schvab-Zeldovich variables and the condition of noncoexistence of the reactants.

Isotherms and streamlines of the flow around a coal particle of diameter 400 microns and 20 mm for Reynolds numbers 0.64 and 31.88 are obtained.

Calculation shows an abrupt separation of the flow at Re = 318.76, leading to a large region of relatively intense and cold recirculating flow that extends downstream.

Among major shortcomings of the model an absence of the temperature and chemical content of the coal particle could be mentioned. The main results of the work concern coal particles of a large diameter range of 0.4–20 mm. The coal particle and flow velocity augmentation leads to the increasing of the gas dynamics influence on the gasification rate of the coal particle.

Author stated that a velocity of 10 m/s would be required for the flow to have a noticeable effect on a particle of radius 40 microns, but such a combination of high velocity and small particle size is not realistic.

A study [22] is devoted to the investigation of the influence of temperature fluctuations of the flow motion for the gas and coal particle on the pyrolysis process.

The instantaneous particle energy equation is expressed as:

$$m_p \cdot c_{m\,p\cdot} \cdot \frac{dT_p}{d\tau} = \pi \cdot d_p \cdot \lambda_{pr} \cdot Nu_p \cdot \frac{k}{e^k - 1} \cdot \left(T_{pr} - T_p\right) + \pi \cdot d_p^2 \cdot \varepsilon_p \cdot \sigma_0 \cdot \left(T_w^4 - T_p^4\right) + G_v \cdot H_v, \quad (36)$$

where H_v – heat of pyrolysis reaction, J/kg; k – constant defined from relationship:

$$k = -\frac{m_p \cdot c_{mp\ pr}}{\pi \cdot d_p \cdot Nu_p \cdot \lambda_{pr}}. \quad (37)$$

The gas instantaneous temperature in the particle energy equation is assumed to take a uniform spatial distribution but vary with time in a simple harmonic way as:

$$T_{pr} = \overline{T}_{pr} \cdot \left[1 + A_T \cdot sin\left(2 \cdot \pi \cdot f \cdot \tau\right)\right], \quad (38)$$

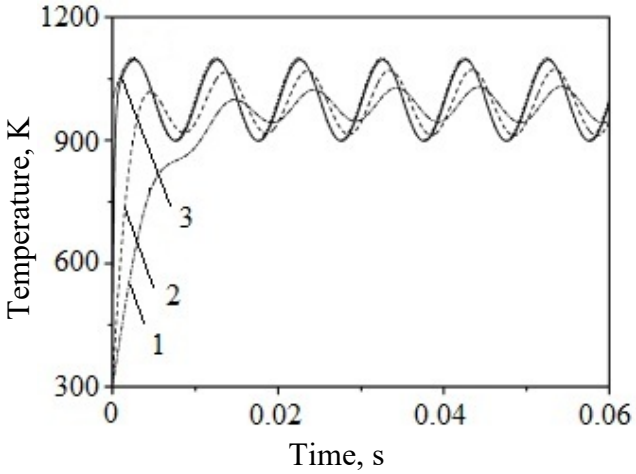
where $\overline{T}_{pr}$ – is the time-averaged gas temperature, K; A_T – is the fluctuation amplitude of the gas temperature.

The fluctuation frequency of the gas temperature fluctuation f is determined by the turbulent time scale, i.e.:

$$f = \frac{1}{\tau_T}, \tag{39}$$

where τ_T – turbulent time scale, s.

The results of experimental and theoretical study proves that for gas temperature of 1000 K and coal particle size range of 10–50 microns gas temperature fluctuations are reached at the level of 900–1100 K (fig. 6).



1 – 50 mkm; 2 – 30 mkm; 3 – 10 mkm

Figure 6 – Instantaneous particle and gas temperature for the time-averaged gas temperature of 1000 K

In work [23] the devolatilization of an isolated coal particle moving relative to the surrounding gas is numerically simulated and assuming that the released volatiles burn in an infinitely thin diffusion flame around the particle or not at all.

The motion of the particle may have an important effect on the shape and position of the flame of volatiles, but it has only a mild effect on the devolatilization process for the particle sizes typical of pulverized coal combustion. This effect increases for large particles or in the absence of radiation.

The relative motion enhances the heat transfer between the particle and the gas, causing the devolatilization time to decrease at high gas temperatures and to increase at low gas temperatures.

Major shortcomings of the model are as follows: uniformity of temperature distribution inside the particle, neglecting of the chemical reactions of devolatilization heat, size decreasing during combustion process.

Study [24] is dedicated to the detailed investigation of coal particle size change influence on the kinetics of the chemical reactions of devolatilization and combustion. It is outlined that after a certain period of time change of the combustion chemical reaction rates and temperature of the coal particle surface no more depends on the initial size of the coal particle.

A decrease of the burning rate with increasing water concentration of the gas phase is observed. Hence, the oxygen diffusion flux is supposed to be the rate limit-

ing factor.

Most integrately gas dynamics and combustion of a coal particle are considered in study [25]. Comparative analysis of six two-equation Reynolds-averaged Navier-Stokes (RANS) models for simulation of a non-swirl coal flame in a pilot-scale furnace has been investigated. Some features of the calculation could be outlined.

Predictions of the standard $k-\varepsilon$ model, RNG $k-\varepsilon$ model, BSL, and SST model are generally in good agreement with the experimental data of the gas phase velocity, its temperature, carbon dioxide and oxygen volume fractions within combustion zone. The Wilcox $k-\omega$ model generally overpredicts oxygen volume fraction and underpredicts carbon dioxide volume fraction that is, probably, due to increased value of turbulent viscosity in vicinity of the burner. The modified $k-\varepsilon$ model yields results that have large discrepancies from measurements.

Study [26] is devoted to the investigation of the volatile flame influence on the combustion process of the char particle. Devolatilization kinetics is described by equation (13). Devolatilization process is describes by equations (9), (11), (12).

Major shortcomings of the model are as follows: spherical shape of the particle is considered, combustion process of the coal particle takes place in quiescent air, volatiles are consist of methane exceptionally.

4. Conclusions

Despite a century of experimental and theoretical investigations in coal particle ignition and combustion process it is still far from its completion.

Analysis and integration of the known mathematical models shows that most scientists focused on separate aspects of the theory but those aspects do not unite all the features of the ignition and combustion processes of the coal particles. Therefore, very often the results of the studies are important only from the theoretical point of view and could be applied for modeling of pulverized coal combustion with significant limitations.

Obviously, new model of the coal particle ignition and combustion should be created. That model has to solve optimization tasks of the ignition and combustion processes as well as take into account integrated approach of the particle heating process, coupled two-phase gas dynamics, kinetics of the chemical reactions. In addition, new mathematical model have to be solved numerically.

The basis and assumptions for new mathematical model are as follows:

- a theory of two-phase flow should be taken into account, however, gas phase continuum is considered as incompressible liquid;
- for calculation of a discrete phase parameters either model of interpenetrating continua or trajectory model could be used.

Initial parameters at the thermal device inlet of the model are considered as raw data, initial gas content is considered as atmospheric air content (nitrogen, oxygen, water steam), initial coal particle content is considered as coal content before combustion (carbon, sulfur, hydrogen, oxygen, water, nitrogen ash and volatiles).

Ways for advancing of mathematical model of pulverized coal ignition and combustion are as follows:

1. A mathematical model has to describe gas dynamics of the turbulent non-isothermal flow by the partial differential equations (equations for conservation of momentum and energy, continuity equation, equations for mass fraction of the chemical constituents). Flow turbulence is taken into account by using one the well-known turbulence models (k–ε model, Spalart-Allmaras model, etc.).

2. Interaction of gas flow with dispersed phase as well as walls of the channel in the equation of the momentum conservation is taken into account by the terms that describe momentum exchange between phases through gas dynamic drag force [27].

Energy conservation equation contains source terms that define convective and radiative heat transfer of the flow with particles as well as heat release of chemical reactions [28].

3. Gas contents change is determined from equations for mass fraction of the chemical constituents. Those equations contain source terms that take into account formation rates of the chemical constituents due to chemical reactions within flow and particles.

Special attention should be paid to the influence of the combustion process on the ecological aspects, in particular, to the nitrogen and sulfur oxides formation.

4. Dispersed phase flow is described by equations that contain gas dynamic drag force and gravity.

5. Energy conservation equation should take into account convective and radiative heat transfer as well as heat of chemical reactions related to the initial chemical constituents.

6. Equations of mass and particle radius reduction should contain terms that describe devolatilization as well as chemical content change due to equations of the chemical reactions rates.

7. The terms in equations that account heterogeneous chemical reactions rates as well as heat and mass transfer between coal particles and gas should consider chemical reactions that take part inside coal particles, porosity, ash content and non-spherical shape of the coal particles.

8. If volume fraction of a discrete phase exceeds critical value 0.02 [29] a mathematical model should be supplemented by equations and amendments for drag force coefficient as well as heat and mass transfer coefficients, etc.

9. Homogeneous and inhomogeneous chemical reactions of devolatilization are subjected to the Arrhenian kinetics.

10. For a stage of coal particles rapid heating a transient heat transfer should be taken into account as well as formation conditions for dynamic and thermal boundary layers.

11. For coal particle Biot number less than 1 temperature change along the particle cross section can be neglected. In this case particle cross section temperature could be calculated as mass-averaged one. For $Bi>1$ a temperature inside coal particle changes significantly that makes a mathematical model more complicated since solution of internal heat transfer problem is necessary.

12. The mathematical model should be supplemented by appropriate boundary conditions as well as approximating relationships for thermophysical properties.

13. For creation of discrete analog for the mathematical model control volume method is used with further realization of SIMPLER algorithm.

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АНАЛІЗ ТА ШЛЯХИ УДОСКОНАЛЕННЯ МАТЕМАТИЧНОЇ МОДЕЛІ ЗАПАЛЮВАННЯ ТА ГОРІННЯ ПИЛОВУГІЛЬНОГО ПАЛИВА

Жевжик О.В., Потапчук І.Ю., Перцевий В.О., Секар М.

Анотація. Представлений аналіз математичних моделей запалювання й горіння окремої частинки, а також вугільної хмари. Наведені й проаналізовані моделі, які враховують наявність у частинках золи, вплив співвідношення кількості вугілля й первинного повітря (коефіцієнта надлишку) і розміру частинок вугілля на процес запалювання. Показане, що спрощення в математичних моделях у більшості випадків призводять до втрати точності розрахунків й тому результати не можуть бать використані для практичних цілей. Моделювання складних процесів підведення повітря з наближенням рівномірності також призводить до сумнівних результатів. Істотний вплив на запалювання й горіння частинок вугілля впливає вміст і інтенсивність виходу летких речовин та хімічні реакції, які відбуваються при цьому. Швидкість виходу летких пропонується розраховувати за законом Арреніуса, а енергію активації й частотний фактор вважати такими, які не залежать від виду вугілля, а визначаються тільки температурою частинки. Урахування теплообміну випромінюванням і зменшення діаметра частинок при горінні позитивно позначається на адекватності отриманих результатах. Є результати, згідно з якими від початкового діаметру частинок вугілля суттєво залежить реакційна здатність і втрати з недопалом. Більшість моделей не враховують зміну температури усередині частинок при нагріванні, запалюванні й горінні в апараті, але є роботи, які спеціально присвячені дослідженню полів температур усередині частинок, а також впливу форми частинок на швидкість згоряння. Моделювання показало, що рух відносно газу приводить до інтенсифікації теплообміну між частинками й навколишнім середовищем, при цьому зменшується час виходу летких речовин при високій температурі навколишнього газу. Відзначається зниження швидкості хімічних реакцій горіння при збільшенні концентрації водяної пари в газоподібному середовищі навколо частки, тобто дифузія кисню є обмежуючим чинником у процесі згоряння частинок. Найбільш повно й фізично вірно газодинаміка при горінні визначається в моделях, де використовуються відомі моделі турбулентності, такі як стандартна k-ε модель, RNG k-ε модель, BSL модель і SST модель. Наприкінці статті викладені концепції вдосконалення моделі запалення й горіння частинок вугілля.

Ключові слова: пиловугільне паливо, горіння, випаровування, частинка, хімічна реакція, займання.