

Effect of the Shape of Particles on the Characteristics of the Ignition of Coal–Water Fuel

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Abstract—A solution to the problem of the ignition of a coal–water fuel particle under the conditions of radiation-convective heat exchange with the environment was proposed. The mathematical simulation was carried out taking into account the combined occurrence of a set of physical and chemical processes (thermal conductivity, the evaporation of water, the thermal decomposition of the organic matter of a coal component, the filtration of water vapor and gaseous thermal decomposition products to the surface, and the chemical interaction of water vapor with the solid and gaseous products of the pyrolysis of coal) in the initial and slightly dried parts of the fuel. The effect of the configuration of a particle on the delay times of ignition was established based on an example of two typical shapes (sphere and cube).

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INTRODUCTION

The development of coal–water power engineering [1, 2] initiates the development of new approaches to solving the problems of the preparation of coal–water fuel (CWF) for combustion. The basic problems of ignition and combustion remain currently unsolved [3–8]. As a rule, experimental data on the ignition of CWF particles [3–5] are represented in the form of the dependences of the delay time of ignition on surface particle temperature or time. Moreover, the experimental studies of the conditions and characteristics of the ignition of coal–water fuel based on a particular coal over a real range of changes in the temperatures of furnace atmospheres are very difficult to perform. The main problem is the measurement of the delay time of the ignition of a single particle against the background of its surrounding flame. Under these conditions, errors in the measurement of any parameters (particle surface temperatures, moments of ignition, and particle sizes) are very large (possibly, even comparable with the measured times). Published results [3–5] are not entirely consistent with each other as a result of different procedures and experimental conditions. Therefore, the theoretical studies of heat transfer in a CWF particle in a period that precedes ignition were carried out with the use of a mathematical model, which differed significantly from known models in the completeness of the description of physical and chemical processes that occur in a CWF particle in the period of thermal preparation [6].

Mathematical models [6–12] developed for describing the ignition of CWF particles contain a number of essential simplifications related to the tentative separation of the entire process into a number of separately occurring interconnected consecutive stages (inert heating, water evaporation, thermal degradation, ignition, and combustion). The process of water removal was described [10–12] in terms of a hypothesis on the equilibrium parameters at the water–steam interface. However, it is necessary to note that the set of physicochemical processes that precede the ignition of fuels is performed simultaneously over the entire time interval before ignition.

The effect of the shape of a particle on the conditions and characteristics of ignition remains the most important problem in the simulation of the combustion of CWF particles. It was experimentally established [13, 14] that particles of various geometric shapes are formed upon the production of a coal–water slurry. As a rule, all of them are irregular polyhedrons saturated with water, the number and size of whose faces vary in a random manner. It is believed that the deformation of a particle [15] upon the crushing of coal and the removal of a water film from its surface [16] (because of the action of aerodynamic forces) lead to different CWF configurations. For these reasons, the simulation of the real shape of CWF particles is difficult to perform. It is believed that the shape of a particle can exert a considerable effect on the characteristics and conditions of CWF ignition [17].

Under the real conditions of fuel preparation at thermal power plants, it is technically complicated to prepare CWF particles of one configuration, whereas a specified combustion mode is possible only with a particular shape of coal–water fuel particle.

Up to now, the shape of coal–water fuel particles in the period of thermal preparation (on heating in a high-temperature atmosphere) is interpreted by different researchers in different ways [10, 13]. In the furnace volume, a CWF particle as a sphere covered with a thin layer of water over the entire surface cannot be set on fire before the complete evaporation of this layer. Under real conditions, ignition occurs only if a dry coal fuel zone is formed; therefore, there is no reason to simulate the process of the ignition of CWF particles of a drop-like or ellipsoid shape. The CWF particle in an induction period (preceding ignition) has the shape of a coal particle, which forms the basis of any element of a coal–water slurry. This particle can be of any shape (tetrahedron, cube, sphere, cone, pyramid, irregular polyhedron, etc.). Therefore, any configuration can be chosen as a base in the theoretical analysis of the conditions and characteristics of CWF ignition (the probabilities of their appearance after grinding differ only slightly from one another). In the numerical simulation, a spherically shaped particle was chosen as a basis. However, in this case, the main goal of the study was to examine the influence of the shape of a particle on the conditions and characteristics of ignition by comparing the results of a simulation of CWF ignition within the framework of a solution of two one-dimensional problems (in the spherical and Cartesian coordinate systems). In spite of the simplification of the geometric formulation of the problem, this comparison is most reasonable because a change to two-dimensional (planar) problems significantly complicates the procedure of the solution of heat and mass transfer problems under the conditions of intense physicochemical transformations.

The aim of this work was to solve the problem of the ignition of a coal–water fuel particle for the two most probable configurations of this particle taking into account the simultaneous occurrence of main physicochemical processes (thermal conductivity, water evaporation, water vapor filtration through the porous structure, thermal decomposition of the organic matter of CWF, thermochemical interaction of combustible components with an oxidizing agent, and ignition) in the porous structure of the fuel.

Formulation of the Problem

The formulation of the problem is different from those developed earlier [5–11] in the fact that the processes preceding the ignition are considered in combi-

nation during an induction period rather than separately in time [6–10] and space [11, 12].

It was assumed that, at the point in time $t = 0$, the CWF particle falls into the typical conditions of the combustion system of a boiler unit. The process of water evaporation is intensified as the fuel temperature is increased. The front of a phase transition penetrates deep into the particle. As a result of the evaporation of water and the filtration of the vapor, two zones are formed. The thermophysical properties of the first zone correspond to the initial CWF. The second zone is a porous coal framework, which includes the organic and inorganic matter of the fuel and water vapor, which is formed as a result of evaporation. Water vapor is filtered through pores under the action of a pressure drop to cool the coal framework, and it enters into thermochemical interaction with carbon. The subsequent heating of CWF initiates the thermal decomposition of the organic matter of fuel with the release of volatile components.

The products of the thermal decomposition of organic matter and the chemical interaction of carbon with water vapor are filtered together with water vapor to the heated surface of the particle, where they form a steam–gas mixture, which is ignited upon reaching the critical values of temperature and fuel concentration.

Within the framework of the above-formulated physical model, the problem of heat and mass transfer in the induction period [20] is described by the system of partial differential equations given below with appropriate boundary conditions.

The mathematical model of ignition for a spherical particle is the following:

thermal conductivity equation for the initial (moist) part of fuel

$$C_1 \rho_1 \frac{\partial T_1(r, t)}{\partial t} = \lambda_1 \cdot \left[\frac{\partial^2 T_1(r, t)}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial T_1(r, t)}{\partial r} \right], \quad (1)$$

$$t > 0, \quad 0 < r < r_v, \quad T \leq T_v;$$

energy equation for the dehydrated part of CWF

$$C_2 \rho_2 \frac{\partial T_2(r, t)}{\partial t} = \lambda_2 \cdot \left[\frac{\partial^2 T_2(r, t)}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial T_2(r, t)}{\partial r} \right] \quad (2)$$

$$- \sum Q_i \cdot W_i - u \cdot C_p \cdot \rho \frac{\partial T_2(r, t)}{\partial r},$$

$$t > 0, \quad r_v < r < r_0, \quad T \geq T_v;$$

filtration equation for water vapor and the gaseous products of thermal decomposition

$$\frac{m \cdot \mu \cdot Z}{K_p} \cdot \frac{\partial p(r, t)}{\partial t} = \left(\frac{\partial p^2(r, t)}{\partial r^2} + \frac{2}{r} \frac{\partial p(r, t)}{\partial r} \right). \quad (3)$$

The rate of pyrolysis was calculated with the use of the expression [17, 18]

$$W_i = (1 - \eta(r, t)) \cdot k_i \cdot \rho_i \cdot \exp\left(-\frac{E_i}{R \cdot T_2(r, t)}\right). \quad (4)$$

The equation of chemical kinetics for the organic matter of fuel takes the form

$$\frac{\partial \eta_2(r, t)}{\partial t} = (1 - \eta_2(r, t)) \cdot k_0 \cdot \exp\left(-\frac{E_i}{R \cdot T_2(r, t)}\right), \quad (5)$$

$$t > 0, \quad r_V < r < r_0, \quad T \geq T_V.$$

The boundary conditions of the fourth kind are fulfilled at the interface of the initial CWF—dry coal system:

$$\lambda_1 \frac{\partial T_1(r, t)}{\partial r} \Big|_{r=r_V-0} - \lambda_2 \frac{\partial T_2(r, t)}{\partial r} \Big|_{r=r_V+0} = Q_V \cdot W_V, \quad (6)$$

$$T_1(r_V, t) = T_2(r_V, t) = T_V.$$

The system of Eqs. (1)–(6) was solved at the following boundary conditions and closure relations:

$$0 < r < r_0, \quad T(r, 0) = T_0,$$

$$p(r, 0) = p_0, \quad \eta(r, 0) = \eta_0,$$

$$-\lambda_2 \frac{\partial T_2(r_0, t)}{\partial r} = \alpha \cdot [T_c - T_2(r_0, t)] + \varepsilon \cdot \sigma \cdot [T_c^4 - T_2^4(r_0, t)] + \sum_i Q_i \cdot W_i, \quad (7)$$

$$\frac{\partial T_1(0, t)}{\partial r} = 0, \quad (8)$$

$$\frac{\partial p(r_V, t)}{\partial r} = \frac{K_p}{v} u(r_V; t), \quad (9)$$

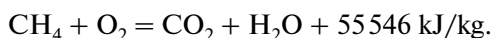
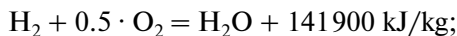
$$p(r_0; t) = p_0. \quad (10)$$

The rate of the reaction $C + H_2O = CO + H_2 - 118.485 \text{ MJ}$ was calculated from the following expression:

$$W_i = k_i \cdot c_i \cdot \rho_i \cdot \exp\left(-\frac{E_i}{R \cdot T_2(r, t)}\right), \quad (11)$$

$$t > 0, \quad r_V < r < r_0, \quad T \geq T_V.$$

It was assumed that the kinetics of interaction of thermal decomposition products with an oxidizing agent and the reaction of water vapor with carbon are responsible for the process of CWF ignition. The following three main reactions at the particle surface were considered:



For determining the rates of these reactions, the following dependence was used [18]:

$$W_i = k_i \cdot c_i \cdot \rho_i \cdot \exp\left(-\frac{E_i}{R \cdot T_2(r_0, t)}\right). \quad (12)$$

The density of gaseous components was calculated from the equation of state

$$\rho_i = \frac{p(r, t) \cdot M}{T(r, t) \cdot R}. \quad (13)$$

The rate of vapor filtration was calculated with the use of the mathematical expression of Darcy's law

$$u = -\frac{K_p \partial p}{\mu \partial r}. \quad (14)$$

The mathematical model that describes heat and mass transfer processes in a cubic particle is an analogous system of equations and boundary conditions written in the Cartesian coordinate system.

The following notation was used: T_0 is the initial temperature of a particle, K; T_c is the ambient temperature, K; r_V is the evaporation front radius, m; r_0 is the external radius of the particle, m; σ is the blackbody radiation constant, $W \text{ m}^2 \cdot K^4$; α is the convective heat transfer coefficient, $W \text{ m}^2 \cdot K$; λ_1 is the thermal conductivity coefficient of the initial part of CWF, $W \text{ m}^{-1} K^{-1}$; λ_2 is the thermal conductivity coefficient of the dry part of CWF, $W \text{ m}^{-1} K^{-1}$; K ; C_1 is the heat capacity of the initial part of CWF, $J \text{ kg}^{-1} K^{-1}$; C_2 is the heat capacity of the dry part of CWF, $J \text{ kg}^{-1} K^{-1}$; W_V is the mass flow rate of water evaporation, $\text{kg m}^{-2} \text{ s}^{-1}$; Q_V is the heat effect of water evaporation, J/kg; Q_i is the heat effect of a chemical reaction, J/kg; k_i is the preexponential factor of a chemical reaction, 1/s; E_i is the activation energy of a chemical reaction, J/mol; u is the rate of filtration of water vapor, m/s; C_p is the specific heat at constant pressure of water vapor, $J \text{ kg}^{-1} K^{-1}$; ρ is the density of a steam—gas mixture, kg/m^3 ; p is the pressure of a vapor phase, Pa; m is the porosity; Z is the degree of compressibility of water vapor, 1/Pa; K_p is the degree of permeability of the porous structure, m^2 ; μ is the dynamic viscosity of water vapor, Pa s; c_i is the concentration of a corresponding component of chemical reaction; and i is the ordinal number of a chemical reaction.

The evaporation boundary coordinate was found from the expression

$$r_V = r_0 - \int_0^\tau u_F \cdot d\tau,$$

where $u_F = \frac{W_V}{\rho_W}$ is the linear velocity of the evaporation front, m/s.

The mass flow rate of evaporation was calculated from the expression [19]

$$W_V = W_0 \cdot \exp\left(\frac{Q_V \cdot M \cdot (T_V - T_0)}{R \cdot T_0 \cdot T_V}\right), \quad (15)$$

where T_V is the temperature at the vaporization boundary, K; T_0 is the temperature of water, which corresponds to a freezing point, K; W_0 is the rate of water evaporation at the temperature T_0 , $\text{kg m}^{-2} \text{s}^{-1}$; M is the molar mass of water vapor, kg/mol ; R is the universal gas constant, $\text{J mol}^{-1} \text{K}^{-1}$; and ρ_W is the density of water, kg/m^3 .

The system of nonlinear differential Eqs. (1)–(15) was solved by the finite-difference method. An iteration algorithm developed for solving heat and mass transfer problems under the conditions of intense phase transformations [20, 21] and high-temperature pyrolysis of composite heatproof polymeric materials [22] was used. Because of the high heating rates of

CWF and large temperature gradients across the particles, the grid steps of a computational mesh with respect to time and the space coordinate were chosen analogously to those published previously [23, 24]. In order to substantiate the reliability of the results of the numerical simulation of the test processes, the conservatism of the difference scheme was checked by a method developed for the analysis of the results of solving the nonlinear problems of the ignition and combustion of condensed substances [25, 26].

In these studies, D coal from the Kuznetsk Basin was chosen as a base material for coal–water fuel [27, 28].

The following technical characteristics and the elemental composition of this coal are given below in the table: W^a , the humidity of fuel; A^d , the ash content; V^r , the content of volatile components; ρ , the density; C^r , the carbon content on a dry ash-free basis; H^r , the hydrogen content on a dry ash-free basis; $N^{\text{daf}} + O^{\text{daf}}$, the sulfur content on a dry ash-free basis; $N^{\text{daf}} + O^{\text{daf}}$, nitrogen and oxygen compounds on a dry ash-free basis.

Technical characteristics and elemental composition of coal

Deposit and coal grade	Technical characteristics				Elemental composition, %			
	W^a , %	A^d , %	V^{daf} , %	ρ_c , kg/m^3	C^{daf}	H^{daf}	S_t^{daf}	$N^{\text{daf}} + O^{\text{daf}}$
Kuznetsk Basin, D coal	6.2	12.1	40.2	1380	77.9	5.3	0.3	15.5

The model of thermophysical properties that takes into account ratios between the volume fractions of components (water, coal, and water vapor) in the wet and dry fuel zones was chosen:

$$\lambda_1 = \varphi_3 \lambda_3 + \varphi_4 \lambda_4, \quad C_1 = \varphi_3 C_3 + \varphi_4 C_4,$$

$$\rho_1 = \varphi_3 \rho_3 + \varphi_4 \rho_4,$$

$$\lambda_2 = \varphi_3 \lambda_3 + \varphi_5 \lambda_5, \quad C_2 = \varphi_3 C_3 + \varphi_5 C_5,$$

$$\rho_2 = \varphi_3 \rho_3 + \varphi_5 \rho_5,$$

where φ is the volume fraction of a corresponding fuel component: 3, water; 4, coal; and 5, water vapor.

As is well known based on coal–water fuel technology [29, 30], the concentrations of a coal component and water vary in ranges from 50 to 70 and from 50 to 30%, respectively. We decided on the ratio between the coal–water system components that is most frequently used in actual practice (60 and 40%, respectively) [31, 32]. We assumed that the presence of additives and plasticizers does not affect the characteristics and conditions of ignition.

According to published data, the possible particle sizes of coal–water fuel vary from $0.05 \cdot 10^{-3}$ [13] to $8 \cdot 10^{-3} \mu\text{m}$ [33]. For the analysis of the characteristics of ignition, we used a range of the most typical sizes from $0.4 \cdot 10^{-3}$ to $1 \cdot 10^{-3} \mu\text{m}$. Many aspects can be considered in the analysis of the applicability of CWF particles with a specific fractional composition. The following three factors are most important:

The first factor is power consumption for the crushing of coal. A twofold decrease in the characteristic sizes of fuel particles leads to an increase in energy consumption by a factor of more than 4 [34]. Therefore, crushing to a characteristic size of several micrometers is very energy consuming. Furthermore, this grinding is a process associated with fire risk (the most up-to-date Ukrainian thermal power plant in Uglegorsk, which burned ultradispersed coal, was completely destroyed by fire as a result of carbon dust ignition).

The second factor is that the ultradispersed particles of CWF lead to the intense erosion of burners

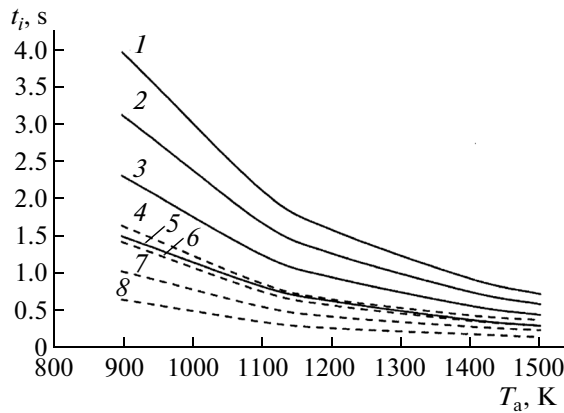


Fig. 1. Dependence of the delay time of ignition on the ambient temperature for particles with the characteristic dimension δ (radius for a sphere): (1) $\delta = 1 \cdot 10^{-3}$ m; (2) $\delta = 0.8 \cdot 10^{-3}$ m; (3) $\delta = 0.6 \cdot 10^{-3}$ m; (5) $\delta = 0.4 \cdot 10^{-3}$ m, a spherical particle; (4) $\delta = 1 \cdot 10^{-3}$ m; (6) $\delta = 0.8 \cdot 10^{-3}$ m; (7) $\delta = 0.6 \cdot 10^{-3}$ m; and (8) $\delta = 0.4 \cdot 10^{-3}$ m, a cubic particle.

[35]. Therefore, grinding to a characteristic size of $0.01 \cdot 10^{-3}$ m is inadvisable.

The third factor—the direct sputtering of a coal–water slurry to particle sizes of $0.01 \cdot 10^{-3}$ – $0.05 \cdot 10^{-3}$ m—is an independent complex technological process, whose results cannot be always predicted in terms of quality criteria. The formation of water drops that do not contain a coal component is possible. Furthermore, power consumption for the preparation of this ultradispersed CWF (not only for grinding but also for mixing) is very high [36].

For the above reasons, the most real sizes were chosen for the analysis of the ignition of CWF particles.

As a result of the numerical simulation, the delay times of ignition (Fig. 1) were determined for the particles of two configurations depending on ambient temperature at different characteristic dimensions δ . A significant difference in the delay times of ignition can be noted for spherical and cubic particles identical in terms of characteristic dimensions. Thus, a cubic particle with the characteristic dimension $\delta = 4 \cdot 10^{-3}$ m in an atmosphere with the temperature $T_a = 900$ K ignited more slowly than a spherical particle with the radius $r_0 = 4 \cdot 10^{-3}$ m by a factor of almost 2.5. The found behaviors can be explained by the higher ability of a sphere (in comparison with a cube) to accumulate thermal energy. Accordingly, an increase in the surface temperature of a spherical particle occurs much more rapidly.

Figure 2 shows the time dependences of the surface temperatures of CWF particles. Each of the particles is characterized by a change in the slope of the temperature curve at the point (T_V, t_V) , which characterizes the point in time of the completion of a water removal process. The thermal conductivity of the dry porous coal framework is much lower than that of the initial CWF, and an increase in the temperature to a critical value occurs considerably more rapidly.

For the determination of the limiting cases of ignition, we also compared the delay times of ignition of CWF particles in an atmosphere with the temperature $T_a = 900$ K and different configurations within the framework of the three versions of concepts of ratios between geometric dimensions in the sphere–cube system. Figure 3 illustrates this comparison. It is obvious that, in any configuration, a cubic particle is

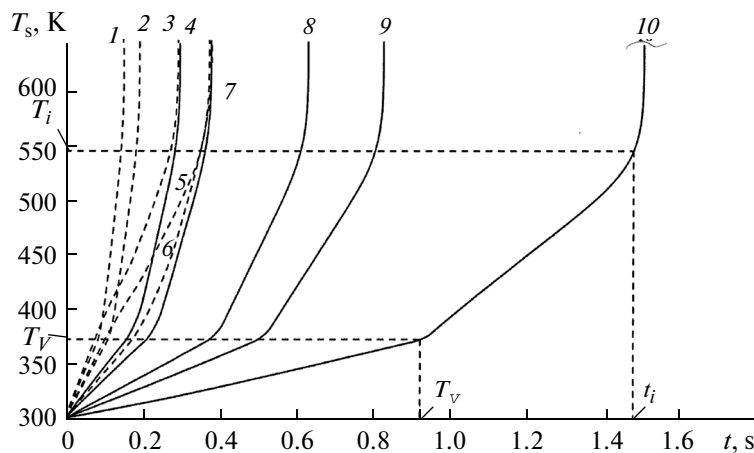


Fig. 2. Dependence of the particle surface temperature T_s on time for particles of different configurations with the characteristic dimension $\delta = 0.4 \cdot 10^{-3}$ m in an atmosphere with the temperature T_a : (1) $T_a = 1500$ K; (2) $T_a = 1400$ K; (3) $T_a = 1200$ K; (5) $T_a = 1100$ K; (6) $T_a = 900$ K, a spherical particle; (4) $T_a = 1500$ K; (7) $T_a = 1400$ K; (8) $T_a = 1200$ K; (9) $T_a = 1100$ K; and (10) $T_a = 900$ K, a cubic particle.

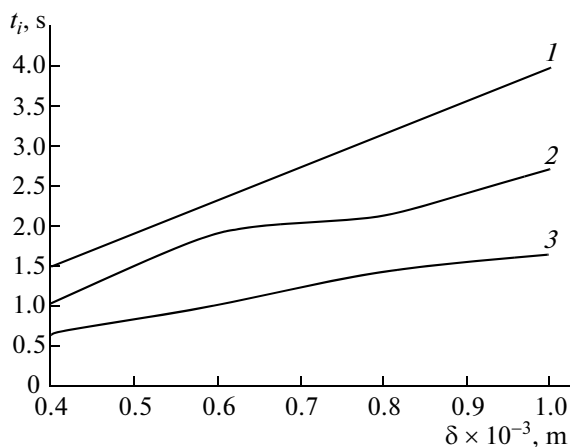


Fig. 3. Dependences of the delay times of the ignition of CWF particles on characteristic dimension at the ambient temperature $T_a = 900$ K: (1) particle in the form of a cube that circumscribes a sphere; (2) particle in the form of a cube inscribed in a sphere; and (3) particle in the form of a sphere.

ignited considerably more slowly than a spherical particle.

The found regularities make it possible to make the conclusion that the shape of a particle plays a determining role in the considered mechanism of ignition. Obviously, a spherical particle is ignited much more rapidly in comparison with a cubic particle. This is related to the increased ability of a sphere to accumulate thermal energy; correspondingly, the surface temperature increases substantially more rapidly.

The experimental results allowed us to conclude that, in the analysis of the conditions and characteristics of ignition of coal–water fuels, it is reasonable to estimate the delay time of ignition with the use of two models of particles (cube and sphere), taking into account the real variety of the possible shapes of CWF particles. In this case, one estimate is an upper-bound estimate and the other is a lower-bound estimate. For the overwhelming majority of other possible configurations, it is most likely that the values of t_i will fall in a range restricted by the values of t_i for a cube and a sphere. This range will increase in proportion to an increase in the particle sizes.

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