

Numerical Simulation of Ignition of Particles of a Coal–Water Fuel

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Abstract: The problem of particle ignition of coal–water fuel has been solved. The simultaneous processes of water vaporization and thermal decomposition of the solid fuel are taken into account. The conditions and characteristics of particle ignition of coal–water fuel under typical furnace conditions were determined by numerical simulation. The obtained values of the ignition delay time are in good agreement with published experimental data.

Keywords: hydrocarbon fuel, ignition, vaporization, thermal decomposition, filtration, volatiles, ignition delay.

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INTRODUCTION

Ignition of coal–water fuel (CWF) particles is a complex of co-occurring physicochemical processes (vaporization, complex heat and mass transfer, thermal decomposition of the solid fuel, chemical interaction of carbon pyrolysis products with steam, oxidation of gaseous fuel components on the particle surface, etc.) [1–12].

According to the results of experimental [1–3] and theoretical [4–9] studies, the basic stages of the ignition of CWF particles are as follows: heating before water vaporization, vaporization, thermal decomposition of the organic part of the CWF with release of gases and the formation of carbon solids, and the reaction of the latter with steam and ambient oxidizer. An approach to the mathematical simulation of the thermal treatment and combustion of CWF particles was developed in [4–7] based on the division of the entire process of ignition into four successive stages. This physical model significantly simplifies the algorithm for solving the general problem and reduces the simulation procedure to the successive solution of four interrelated problems of heat transfer with consideration of one dominant phys-

ical or chemical process in each problem. The approach of [4–7] allows obtaining an approximate solution for each identified stage based on a theoretical analysis of the preceding stage [8, 9].

At the same time, if the characteristic size of the coal–water fuel particles is large enough, all of the above-mentioned processes, i.e., heat conduction, vaporization, filtration of steam in the porous structure of the particle, thermal decomposition of the organic part of the CWF, thermochemical interaction of the fuel components with oxidizers, and ignition, can proceed simultaneously.

The aim of this work is to solve the problem of particle ignition of coal–water fuel using a model that takes into account the main factors and processes.

FORMULATION OF THE PROBLEM

According to [10, 11], a CWF particle is characterized by increased reactivity (and hence reduced ignition temperature as compared with coal). For example, an anthracite-based water-coal particle is ignited at 425–440°C, and a dry particle of coal of the same brand is ignited at a temperature of 800–1000°C. In [10], this is explained by the chemical reaction between steam and coal to form low-reactive complexes [1, 3] which accelerate the oxidation of the organic part of the fuel.

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A coal-water fuel particle usually is an irregular polyhedron, the number of faces in which changes randomly depending on many factors (type of coal, mineral content of the components, grinding technology of the starting solid fuel, storage conditions, et al.). For these reasons, simulation of the actual configuration of a CWF particle is extremely difficult. However, one possibility is a spherical particle model. The probability of this configuration is no more and no less than that all the others [12], so that it can be considered fairly typical and used in the formulation of the problem.

In the most general case, a CWF particle is a multi-component porous structure (water, organic part, mineral part) with pores filled with water.

In the theory of thermal and fire protection, use is made of mathematical models of heat and mass transfer and physicochemical transformations [13, 14] in heat and fire resistant materials under intense heating at high temperature. But models of the type of [14] are too complex to implement and can be used to solve the problems in question only for materials with known characteristics (thermal, thermochemical, physicochemical) in a wide range of temperature (from the initial state to the complete thermal decomposition of the organic part).

In this paper, the formulation of particle ignition problem differs from known formulations [1–12] in that heat and mass transfer processes are not described discretely in time, as in [4–7], or in space, as in [8, 9], but are considered continuously throughout the period of time before ignition and throughout the thickness of the particle.

It was assumed that at the initial time ($t = 0$), a CWF particle enters a high-temperature gas medium and is heated by convection and radiation. Accordingly, the particle begins to vaporize, and as the CWF is heated, the vaporization front moves from the heating surface into the interior of the particle. This results in the formation of a porous layer of dry fuel, in which the temperature at each point increases with time. The vaporized moisture is filtered through the porous carbon skeleton that formed. Steam reacts with carbon (formed after the completion of moisture release) with heat absorption. Upon reaching the condition on the particle surface $T_s \geq T^*$ (T_s is the temperature of the particle surface, T^* is the temperature of decomposition of dry coal) the organic part of the fuel begins to decompose. With further heating and increase in the temperature at each point of the particle, the front $T(r, t) = T^*$ moves deeper into the CWF. This results in the formation of the fuel structure that can be divided into three characteristic zones (I–III in Fig. 1) corresponding to water-saturated fuel (initial state); dry coal at a tem-

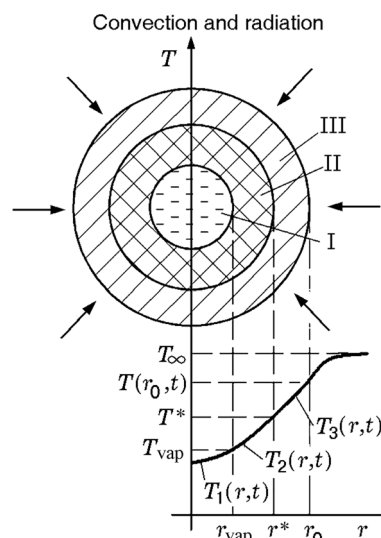


Fig. 1. Schematic diagram of the solution of the problem: I is the zone corresponding to the water-saturated fuel (initial state), II is the zone corresponding to dry coal at a temperature below T^* , and III is the zone corresponding to thermally decomposing dry coal.

perature less than T^* ; thermally decomposed dry coal at a temperature above T^* .

Products of thermal destruction and chemical interaction of the solid carbon residue and steam are blown into the near-wall region to form a gas mixture which is ignited upon reaching the critical temperature and concentration (see Fig. 1).

In the solution of problem (1)–(15) (see below), the thermal characteristics are calculated for each zone based on its physical state and the time variation of the boundaries between the zones.

The following ignition conditions were assumed: the heat generated by the oxidation reaction product of the thermal decomposition and gasification exceeds the heat transferred from the ambient medium; at the interface between the CWF particle and the high-temperature medium, $\frac{dT}{dr} = 0$.

MATHEMATICAL FORMULATION OF THE PROBLEM

The nonstationary differential equations of heat conduction corresponding to the above physical model has the following form:

the energy equation for the initial (wet) part of the fuel [15]:

$$c_1 \rho_1 \frac{\partial T_1(r, t)}{\partial t} = \lambda_1 \left[\frac{\partial^2 T_1(r, t)}{\partial r^2} + \frac{2}{r} \frac{\partial T_1(r, t)}{\partial r} \right], \quad (1)$$

$$t > 0, \quad 0 < r < r_{\text{vap}}, \quad T \leq T_{\text{vap}};$$

the energy equation for the dehydrated part of the CWF [15]:

$$c_2(r) \rho_2(r) \frac{\partial T_2(r, t)}{\partial t} = \lambda_2(r) \left[\frac{\partial^2 T_2(r, t)}{\partial r^2} + \frac{2}{r} \frac{\partial T_2(r, t)}{\partial r} \right] - \sum Q_i W_i - u_{\text{steam}} c_{p, \text{steam}} \rho_{\text{steam}} \frac{\partial T_2(r, T)}{\partial r}, \quad (2)$$

$$t > 0, \quad r_{\text{vap}} < r < r_0, \quad T \geq T_{\text{vap}};$$

the equation of chemical kinetics for the organic part of the fuel [16]:

$$\frac{\partial \eta_2(r, t)}{\partial t} = (1 - \eta_2(r, t)) k_0 \exp\left(-\frac{E}{RT_1(r, t)}\right), \quad (3)$$

$$t > 0, \quad r_{\text{vap}} < r < r_0, \quad T \geq T_{\text{vap}};$$

equation of filtration for steam and the gaseous products of thermal decomposition [17]:

$$\frac{m \xi Z}{K_P} \frac{\partial p_{\text{steam}}(r, t)}{\partial t} = \left(\frac{\partial p_{\text{steam}}^2(r, t)}{\partial r^2} + \frac{2}{r} \frac{\partial p_{\text{steam}}(r, t)}{\partial r} \right), \quad (4)$$

$$t > 0, \quad r_{\text{vap}} < r < r_0, \quad T \geq T_{\text{vap}}.$$

At the interface between the initial CWF and dry coal, the following boundary condition of the 4th kind is satisfied:

$$\lambda_1 \frac{\partial T_1(r, t)}{\partial r} \Big|_{r=r_{\text{vap}}-0} - \lambda_2(r) \frac{\partial T_2(r, t)}{\partial r} \Big|_{r=r_{\text{vap}}+0} = Q_{\text{vap}} W_{\text{vap}}, \quad (5)$$

$$T_1(r_{\text{vap}}, t) = T_2(r_{\text{vap}}, t) = T_{\text{vap}}.$$

System (1)–(4) was solved with the following boundary conditions and closing relations [15–19]

$$0 < r < r_0, \quad T(r, 0) = T_0, \quad p(r, 0) = p_0, \quad (6)$$

$$\eta(r, 0) = \eta_0;$$

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

$$\frac{\partial T_1(0, t)}{\partial r} = 0, \quad (7)$$

$$\frac{\partial p(r_{\text{vap}}, t)}{\partial r} = \frac{\nu}{K_P} u_{\text{steam}}(r_{\text{vap}}, t), \quad (8)$$

$$p(r_0, t) = p_0. \quad (9)$$

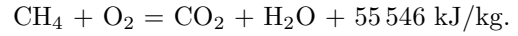
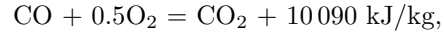
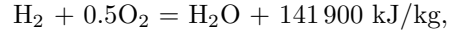
By analogy with [17], the rate of the reversible reaction $\text{C} + \text{H}_2\text{O} = \text{CO} + \text{H}_2 - 118.485 \text{ MJ}$ was calculated by the expression

$$W_i = C_i \rho_i k_i \exp\left(-\frac{E}{RT(r, t)}\right). \quad (10)$$

The pyrolysis rate was calculated by the relation [17]

$$W_{\text{pyr}} = (1 - \eta(r, t)) \rho_i k_i \exp\left(-\frac{E}{RT(r, t)}\right). \quad (11)$$

Ignition of the CWF is a heterogeneous process [15] determined by the kinetics of ignition of the thermal decomposition products and steam–carbon interaction. On the surface of the particle, the following reactions occur:



The rates of these reactions were determined using the relation [19]

$$W_i = k_i C_i \rho_i \exp\left(-\frac{E}{RT(r_0, t)}\right), \quad (12)$$

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

$$\rho_i = \frac{p(r, t) \mu}{T(r_0, t) R}. \quad (13)$$

The filtration rate of steam through the porous structure was determined from the Darcy law

$$u_{\text{steam}} = -\frac{K_P}{\nu} \frac{\partial p_{\text{steam}}}{\partial r}. \quad (14)$$

In (1)–(14) the following notation is used: T_0 is the initial temperature of the particle, T_∞ is the ambient temperature, r_{vap} is the radius of the vaporization front, r_0 is the outer radius of the particle, σ is the blackbody radiation constant, α is the convective heat transfer coefficient, c_1 is the specific heat of the initial part of the WCF, c_2 is the specific heat of the dry part of the CWF, λ_1 is the thermal conductivity of the initial part of the WCF, λ_2 is the thermal conductivity of the dry part of the WCF, W_{vap} is the mass flow rate of water vaporization, Q_{vap} is the

thermal effect of water vaporization, Q_i is the standard enthalpy of formation, k_i is the preexponent of the chemical reaction ($k_{\text{H}_2\text{O}+\text{C}} = 5.6 \cdot 10^{12} \text{ s}^{-1}$ [19], $k_{\text{coal} \rightarrow \text{CH}_4} = 212 \text{ s}^{-1}$, $k_{\text{CO}+0.5\text{O}_2} = 1.4 \cdot 10^{12} \text{ s}^{-1}$, $k_{\text{H}_2+0.5\text{O}_2} = 2.137 \cdot 10^{14} \text{ s}^{-1}$, $k_{\text{CH}_4+\text{O}_2} = 5.6 \times 10^{12} \text{ s}^{-1}$ [20]), E the activation energy of the chemical reaction ($E_{\text{H}_2\text{O}+\text{C}} = 36.207 \cdot 10^3 \text{ J/mol}$ [19], $E_{\text{coal} \rightarrow \text{CH}_4} = 60.6 \cdot 10^3 \text{ J/mol}$, $E_{\text{CO}+0.5\text{O}_2} = 96.8 \times 10^3 \text{ J/mol}$, $E_{\text{H}_2+0.5\text{O}_2} = 129.8 \cdot 10^3 \text{ J/mol}$, $E_{\text{CH}_4+\text{O}_2} = 103.8 \cdot 10^3 \text{ J/mol}$ [20]), u_{steam} is the rate of filtration of steam, $c_{p,\text{steam}}$ is the isobaric heat capacity of steam, ρ_{steam} is the steam density, p_{steam} is the steam pressure inside the particle, m is porosity of the particles, Z is the degree of compressibility of steam, K_P is the permeability of the porous structure, μ is the molar mass of water, ν is the dynamic viscosity of water vapor, C_i is the concentration of the corresponding component of the chemical reaction, i is the serial number of a component of the chemical reaction, and R is the universal gas constant.

The coordinate of the vaporization boundary was determined from the expression

$$r_{\text{vap}} = r_0 - \int u_l d\tau,$$

where $u_l = W_{\text{vap}}/\rho_l$ is the linear speed of propagation of the vaporization front. The mass vaporization rate was calculated by the formula [21]

$$W_{\text{vap}} = W_0 \exp\left(\frac{Q_{\text{vap}}\mu_{\text{steam}}(T' - T_{l0})}{RT_{l0}T'}\right), \quad (15)$$

where T is the temperature at the vaporization boundary T_{l0} the liquid temperature corresponding to the freezing point, W_0 the rate of vaporization at T_{l0} , and μ_{vapor} the molar mass of steam.

SOLUTION METHOD AND INITIAL DATA

The system of differential equations (1)–(10) was solved by a finite difference method with a four-point implicit difference scheme [22, 23]. The chemical kinetics equation (3) was solved by successive approximations. The nonlinear differential equations were solved by iterations using an algorithm developed for problems of ignition of solid fuels under local heating [24, 25]. The results of the numerical simulation were verified by testing the conservativeness of the difference schemes using the method employed in the analysis of the reliability of the results of solution of the problem of ignition of liquid fuels under local heating [25].

The initial data for the calculation were as follows: $T_0 = 293 \text{ K}$, $T_\infty = 1400 \text{ K}$, $p_0 = p_{\text{atm}} = 101325 \text{ Pa}$, $\eta_0 = 0$.

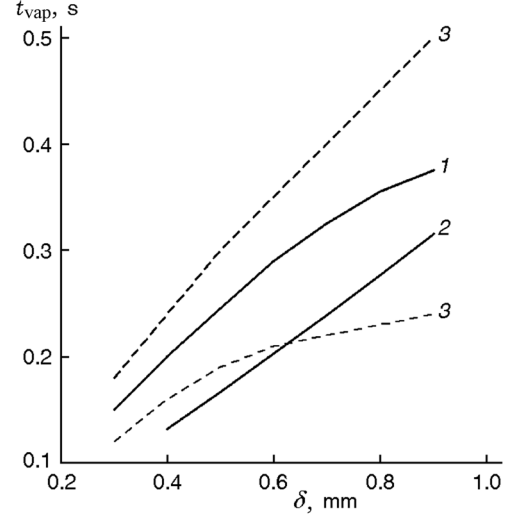


Fig. 2. Dehydration time versus characteristic particle size at ambient temperature $T_\infty = 1400 \text{ K}$: (1) experiment [27]; (2) data of numerical calculation of system (1)–(11); (3) boundaries of the region of scattering of experimental data [27].

The base material for coal–water fuel was assumed to be the D brand coal from the Kuznetsk Basin [26].

Thermal properties of the wet and dehydrated parts of the fuel were calculated taking into account the volume fractions φ of the fuel components:

$$\lambda_1 = \varphi_3\lambda_3 + \varphi_4\lambda_4,$$

$$\lambda_2 = \varphi_4\lambda_4 + \varphi_5\lambda_5 + \varphi_6\lambda_6,$$

where the subscript 3 refers to water, 4 to coal at a temperature below T^* , 5 to thermally decomposing coal at a temperature higher than or equal to T^* , and 6 to air.

RESULTS AND DISCUSSION

The characteristic times of the main stages of the multistage process of ignition of a CWF particle of diameter $\delta = 400\text{--}900 \mu\text{m}$ were analyzed.

Figure 2 shows the characteristic vaporization times $t_{\text{vap}} = \varphi(T_\infty, \delta)$ obtained by numerical solution of Eqs. (1)–(11) and experimental data [27]. Analysis of the results of the numerical simulation shows that for a particle size of $600\text{--}900 \mu\text{m}$, the rate of removal of moisture from the CWF particle can be calculated with a sufficiently high degree of confidence.

Figure 3 shows a comparison of the ignition delays in the system of a CWF particle and a high-temperature medium obtained by solving Eqs. (1)–(11) and in experiments [27]. The deviation of the theoretical values

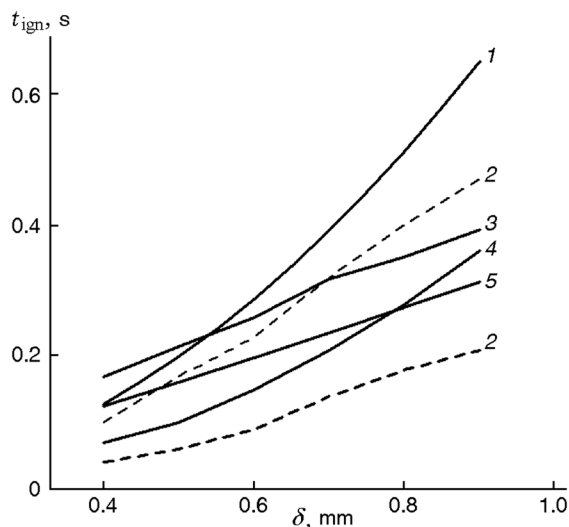


Fig. 3. Ignition delay versus characteristic CWF particle size at ambient temperature $T_{\infty} = 1400$ K: (1) empirical formulas [27]; (2) boundaries of the range of scattering of experimental data [27]; (3) numerical solution of (1)–(11); (4) experiment [27]; (5) numerical solution of (1)–(11) neglecting the effects of vaporization of moisture and pyrolysis of the dry part of the fuel.

from the experimental values for a CWF particle diameter $\delta = 700\text{--}900 \mu\text{m}$ is within the error of the experiment [27]. However, for a particle diameter $\delta < 700 \mu\text{m}$, the deviation of the numerical simulation results is beyond the error limit.

The results suggest that the mathematical model (1)–(11) describes the ignition characteristics of large CWF particles (with a characteristic size over $700 \mu\text{m}$) with reasonable confidence.

The theoretical results presented in Fig. 3 indicate that the use of simplified models of water vaporization [11] to describe heat and mass transfer in a water-coal particle under typical furnace space conditions can lead to large deviations in determining the ignition characteristics. The porous carbon framework resulting from vaporization slows heat transfer, thus reducing the rates of vaporization and thermal decomposition. In other words, the characteristic times of coal pyrolysis and attainment of a high particle surface temperature are substantially increased. Dependences of the ignition delay on the ambient temperature for different diameters [15] of CWF particle spray obtained by numerical solution of system (1)–(11) are shown in Fig. 4.

Analysis of the results (see Fig. 4) shows that the dependences $t_{\text{ign}} = \varphi(T_{\infty}, \delta)$ differ substantially from similar dependences for ordinary solid condensed materials [19] that reflect the exponential relationship between the rate of the chemical reaction of ignition and

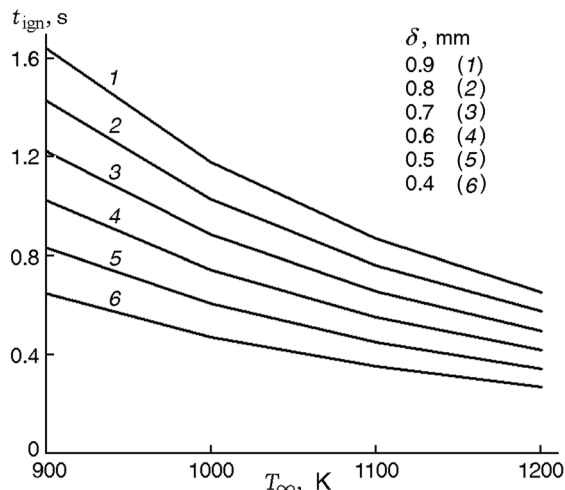


Fig. 4. Ignition delay of particles of different diameters under different heat transfer exchange.

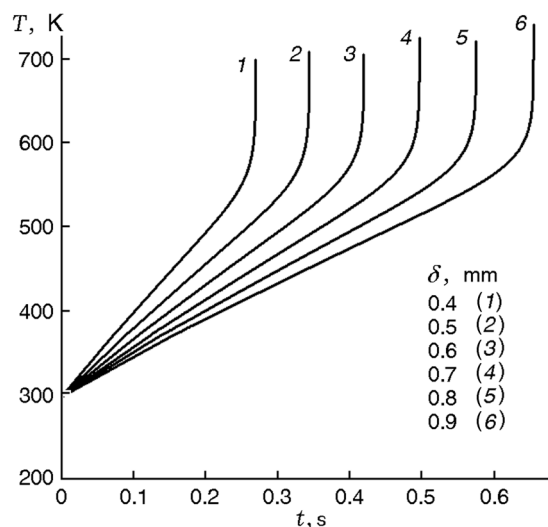


Fig. 5. Surface temperature of particles of different diameters versus time ($T_{\infty} = 1200$ K).

temperature. This is most likely due to the influence of the vaporization of moisture, filtration of steam to the heating surface and its penetration into the near-wall region of the particle. All these physical processes prevent temperature rise in the CWF ignition zone and reduce the concentration of gaseous products of pyrolysis of coal (main fuel). That is, the CWF particle ignition regime is not kinetic (as defined by [19]). Nor can it be classified as a diffusion regime [19]. Most likely, the curves of $t_{\text{ign}} = \varphi(T_{\infty}, \delta)$ illustrate the ignition mode of a coal–water fuel particle resulting from the co-occurrence of a set of interrelated physical processes (heat conduction, vaporization, vapor filtration,

blowing of steam into the near-wall region) and chemical processes (thermal decomposition of coal, the reaction of steam with the coke carbon formed during pyrolysis, the reaction of the gaseous products of thermal decomposition of coal with the ambient oxidizer).

Figure 5 shows time dependences of the CWF particle surface temperature for different particle diameters at the moment of ignition. It is clearly seen that in the range $\delta = 0.4\text{--}0.9$ mm, the maximum values of T_{ign} during ignition do not exceed 620 K.

Increase in the ignition delay time with increasing particle diameter is likely due to the need for complete vaporization of water. Comparison of Figs. 2–4 suggests that ignition occurs only after complete removal of all moisture from the porous structure of the coal-water fuel.

CONCLUSIONS

A mathematical model for the ignition of a coal-water fuel particle fuel has been developed that differs from available models [1–12] in the description of the physicochemical processes preceding ignition.

A new approach to the simulation of moisture transfer processes in the porous structure of a high-temperature medium has been proposed that differs in the physical interpretation of moisture vaporization (direct identification of the vaporization front) from the most widely used approach in the theory of high-temperature physicochemical transformations (moisture potential model [28]).

Agreement between the results of the numerical simulation (dependences of the ignition delay on the ambient temperature and CWF particle size) and experimental data [27] indicates that the basic physical propositions developed in creating the general theory of ignition of condensed materials [14] are suitable for describing the process considered.

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