# Influence of the degree of coal metamorphism on characteristics and conditions of ignition of coal-water fuel drops[*]

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The results of theoretical studies of the processes of ignition of water-coal fuel droplets based on brown coal, semi-anthracite, anthracite, long-flame and fat coal under the conditions corresponding to the combustion spaces of typical modern boilers are presented. The influence of the degree of metamorphism (structural-molecular transformation of organic matter of coal) and concentration of the organic component of the base fuel (coal) on the conditions of ignition of water-coal fuel particles is analyzed. It is determined that the type and grade of coal have a significant impact on the dynamics of fuel ignition. It was shown that in the case of ignition of coal-water fuel made of mineral coal, the ignition of particles based on semi-anthracite and anthracite is the fastest (by 20%), and ignition of coal-water fuels of fat coal is the slowest. The latter is explained by the lower heat capacity and thermal effect of pyrolysis of this fuel, as well as the relatively high heat conductivity of anthracite coal as compared to fat coal. It has been determined that drops of coal-water fuel made of brown coal ignite substantially (2 times) faster than drops prepared from coal of coal-water particles. This is due to the high content of volatiles in the composition of brown coal.

Comparative analysis of the main characteristics of the process: ignition delay times ($t_{ign}$) obtained by mathematical modeling and experiments showed a satisfactory agreement between the theoretical and experimental values of $t_{ign}$.

**Key words:** coal-water fuel, degree of coal metamorphism, grade of coal, ignition of coke, ignition of volatiles, diffusion of pyrolysis products.

### Introduction

First, ecological, and second, obvious economic prospects of using coal-water fuel (CWF) as the main fuel for thermal power plants were justified many years ago [1]. However, despite this, until now the CWF technology has not become the mainstream even in China power system, where the level of atmospheric pollution with anthropogenic products of solid fuel combustion is extremely high [2, 3]. This relates to a number of objective and subjective reasons. A significant shift in the fuel and energy balance towards the consumption of gas or heavy refinery products (fuel oil) at thermal power plants [4] can be attributed to the subjective

reasons. The tendency of "gasification" of heat and power engineering is caused, first of all, by the price advantages of gas fuel in comparison with coal [5]. Analysis of the use of natural gas in modern industrial production in developed countries shows that the most beneficial for the economic development of any country is not gas burning, but using it as a raw material for the chemical industry [6, 7].

Based on the analysis of numerous publications on the problems of CWF combustion presented in recent years in the world scientific periodicals (for instance, see [3]), it can be concluded that the main objective reason for the small amount of CWF in the overall balance of heat and power generation (these technologies are most common in China, Japan, and USA) can be called the lack of knowledge about the processes of ignition and combustion of such substantially heterogeneous suspension fuels. The currently developed mathematical models of varying degrees of complexity [8–14] and methods for solving the problems of CWF particle igniting [15–19] do not allow comprehensive prognostic modeling of ignition of such fuels, liquid (essentially) in the initial state. Mathematical models of ignition, as a rule, are based on significant assumptions. For example, the mathematical models of [8–10] are based on solving equations, which were written assuming that the temperature field of a particle is uniform, and evaporation occurs on the surface of a fuel particle. In [8], analytical expressions were obtained for calculating the characteristics and conditions of CWF ignition. In a later work [11], it was found that the use of such models is possible only in the case of burning the particles of ultra-small dispersion ($\delta \leq 1 \cdot 10^{-4}$ m).

Significantly more complex mathematical models developed in [12–15] were formulated under the assumption of discretization of the entire thermal preparation process into a number of sequential and interrelated stages: inert heating, water evaporation, fuel pyrolysis, ignition of coke carbon. However, almost all main processes of heat and mass transfer in a CWF particle occur during the induction period together (at least, after complete evaporation of moisture). Accordingly, it can be said that the use of models [12–15] can lead to significant errors in calculation of the integral characteristics of the process of CWF drops ignition: times of ignition delay.

One of the most comprehensive mathematical models, which takes into account the main physical processes, was proposed in [16]. It is a system of nonstationary partial differential equations that takes into account the basic processes of thermal preparation of fuel that occur together during the induction period under the conditions of intense phase (water evaporation) and thermochemical (thermal decomposition, interaction of water vapors and carbon of coke, ignition of volatiles) transformations. Using model [16], we have analyzed the effect of a fairly large group of the main factors important for calculating the ignition delay time (heat transfer conditions [17], particle shape [18], coal concentration in CWF [19], heterogeneity of porous fuel structure [20]) on the conditions and characteristics of ignition of coal-water fuel. When solving problems [16–20], it was assumed that the process of volatile ignition proceeded directly on the surface of fuel. The changes in concentration of pyrolysis products in time and space in a small neighborhood of particle were not simulated. At the same time, it is known from [21] and [22] that during ignition of solid fuels, diffusion plays the main role in initiating the combustion of combustible gases.

In some mathematical models, it is possible to distinguish formulation of [23], which describes the process of ignition of a water-coal particle in the gas phase. This takes into account evaporation of water, thermal decomposition of the organic part of coal, devolatization and diffusion of pyrolysis products in the external gaseous medium. However, the phase transition (vaporization) is considered in the framework of hypothesis of process equilibrium. At the same time, it was previously determined [24] that the rate of liquid evaporation depends on the temperature of phase transition front and concentration of vapors near the vaporization surface. It is also known [25] that the ignition characteristics of coal are significantly influenced by the degree of metamorphism (black or brown coal), grade and deposit of coal. Constructive substantiation of the choice of sizes and layout of the main components of boilers is carried out,

as a rule, based on the results of determining the characteristics of ignition and combustion of the used solid fuel. However, the above mathematical models [16–20, 23] do not take into account a group of significant thermochemical factors affecting the characteristics of the ignition process. The latter, in particular, include: volatile content in fuel ($M_0$), their composition and properties. It is known [26] that these characteristics of coal can differ significantly depending on the degree of metamorphism, grade and location of a solid fuel deposit.

Based on the analysis of the state of the problem of simulating the ignition of water-coal fuels, we can conclude that the development of a mathematical model of ignition of CWF particles, which takes into account the complex of processes occurring together during the induction period, and individual thermochemical characteristics of the basic component of fuel (coal) is an urgent and unresolved task.

The goal of this work is to perform mathematical modeling of heat and mass transfer processes that occur together during ignition of a coal-water particle and analyze the influence of individual characteristics of coal (thermal characteristics, heat of thermal decomposition, volatile content, etc.) on the conditions of ignition of the drops of coal-water fuel.

### Problem statement

#### *Physical statement of the problem*

When formulating the problem, the model [20], including a set of basic physical processes determined during experimental studies of ignition of water-coal fuel particles, was taken as the basic one. A physical model of the ignition process, which takes into account the basic heat and mass transfer processes occurring under the conditions of intense phase (water evaporation) and thermochemical (thermal decomposition, thermochemical interaction of coke carbon and water vapor, ignition) transformations during the induction period, was formulated.

It was assumed that in accordance with the conditions of fuel combustion in the furnaces of steam boilers, the CWF particle is introduced into the high-temperature oxidizing medium (air) and heated by convection and radiation. As a result of heating, water evaporates intensively. The evaporation front shifts with time from the heating surface into the fuel. As a result, a porous coal frame with high thermal resistance is formed. Water vapors formed during evaporation are filtered through a layer of dry fuel, entering into thermochemical interaction with coke carbon, and form combustible gaseous products of this reaction ($CO$ and $H_2$). A further increase in the particle temperature leads to thermal decomposition of the organic part of coal and release of volatiles, which, together with water vapors and gaseous products of their thermochemical interaction with carbon, are filtered to the heated surface of the fuel particles and injected into the external environment. As a result, a mixture of water vapors, air and various gases with significant concentration gradients is formed in the near-wall region. When reaching the critical values of temperature and mass ratio of volatiles and oxidant, this mixture is ignited. The thermal effect of the volatiles flame initiates the burning of coke carbon of CWF.

It is known [27] that at thermal decomposition of coal, a gas mixture, whose chemical composition depends essentially on a group of factors such as the degree of coal metamorphism, humidity, and deposit, is formed. The composition of volatile components considered as a base when solving the problems is given in Table 1.

#### *Mathematical statement of the problem*

The mathematical formulation of the problem of CWF ignition corresponding to the above physical model includes a system of nonstationary differential equations.

**Composition of gaseous products of pyrolysis [28]**

| Component | Component content, % | |
|---|---|---|
| | Brown coal | Coal |
| Carbon dioxide ($CO_2$) | 15.5 | 2.3 |
| Carbon monoxide (CO) | 15.0 | 5.7 |
| Methane ($CH_4$) | 20.5 | 65.9 |
| Hydrogen ($H_2$) | 25.6 | 18.6 |
| Nitrogen ($N_2$) | 23.4 | 7.5 |

The area of solving the problem is "CWF particle−gas environment" (Fig. 1). During the period of thermal preparation, a drop of CWF can be divided into two zones: initial (saturated with moisture) fuel and dry coal frame. Temperature distribution in such a heterogeneous system is described by the energy equation. It takes into account the removal of moisture, thermal destruction, interaction of water vapor and carbon of coke as well as filtration heat and mass transfer:

$$\frac{\partial H_{cwf}}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\lambda_{cwf}\frac{\partial T}{\partial r}\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\frac{\sin\theta}{r}\lambda_{cwf}\frac{\partial T}{\partial\theta}\right) - \frac{Q_{eva}\,W_{eva}}{h_{spr}}\delta\left(r_{eva},\theta_{eva}\right) -$$

$$-\left[\sum_{i=1}^{2}Q_i\,W_i + C_s\rho_s\left(U_s\frac{\partial T}{\partial r} + V_s\frac{1}{r}\frac{\partial T}{\partial\theta}\right)\right]\cdot\Phi\left(r - r_{eva}, \theta - \theta_{eva}\right), \tag{1}$$

where $\sum_{i=1}^{2}Q_i\,W_i = Q_{c\to vol}\cdot W_{c\to vol} + Q_{C+H_2O}\cdot W_{C+H_2O}$, $H_{cwf} = C_{cwf}(r,\theta,t)\cdot\rho_{cwf}(r,\theta,t)\cdot T(r,\theta,t)$,

$\delta$ is the Dirac function, $\Phi$ is the Heaviside function, $T$ is the temperature, $H_{wcf}$ is the enthalpy; $\lambda_{cwf}$, $C_{cwf}$, and $\rho_{cwf}$ are the heat conductivity coefficient, the heat capacity, and the density of coal-water fuel, respectively; $U_s$ and $V_s$ are, respectively, the radial and azimuthal velocities of water steam and gaseous products of coal thermal decomposition; $C_s$ and $\rho_s$ are the heat capacity and density of water steam; $Q$ and $W$ are the thermal effect and the rate of chemical reaction. The thermal-physical characteristics ($\lambda_{cwf}$, $C_{cwf}$, and $\rho_{cwf}$) are calculated taking into account the evaporation front position. Mass rate of evaporation was calculated from relationship [29]:

$$W_{eva} = W_{fp}\exp\left[\frac{Q_{wat}M_{wat}\left(T\left(r_{eva},\theta_{eva}\right) - T_{fp}\right)}{R\,T_{fp}\,T\left(r_{eva},\theta_{eva}\right)}\right], \tag{2}$$
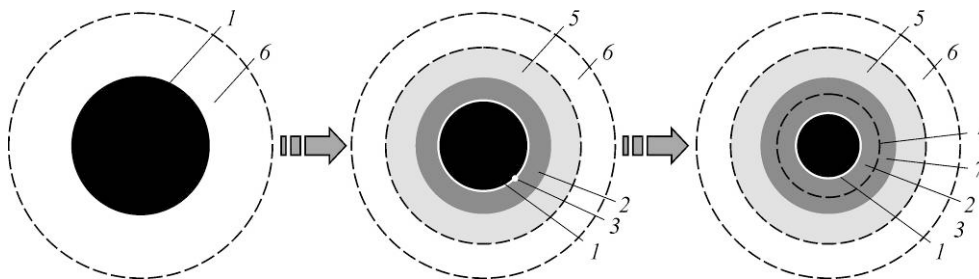


*Fig. 1.* Scheme of problem solving area.
*1* — CWF particle, *2* — layer of dry coal, *3* — "initial CWF – dry fuel layer" interface,
*4* — "dry coal – coal at $T > T_{std}$" interface, *5* — area of interaction between
pyrolysis products and oxidant, *6* — high-temperature gas, *7* — coal at temperature $T > T_{std}$.

where $Q_{wat}$ is the thermal effect of water evaporation, $M_{wat}$ is the molar mass of water, $R$ is the universal gas constant, $T_{fp}$ is the temperature of a triple point of water state (273.16 K). The coordinate of evaporation front was determined from relationship

$$r_{eva} = r_{out} - \int_0^t u_F\, dt, \tag{3}$$

where $u_F = W_{eva}/\rho_{wat}$ is the liner velocity of evaporation front motion, $\rho_{wat}$ is the water density.

When formulating the problem, it was taken into account that water vapors together with the products of thermal decomposition move through a porous carbon frame. The distribution of pressure $p$ along the particle radius was calculated by solving the piezoconductivity equation

$$\frac{\partial(P_f p)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{K_p}{\mu\beta}\frac{\partial p}{\partial r}\right) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\frac{\sin\theta}{r}\frac{K_p}{\mu\beta}\frac{\partial p}{\partial\theta}\right) + \frac{1}{\rho\beta}\sum_{i=1}^3 f_i, \tag{4}$$

where $\displaystyle\sum_{i=1}^3 f_i = \frac{1}{s}\left[\left(s W_{c\to vol} + W_{C+H_2O\to CO+H_2}\right)\Phi\left(r - r_{eva}, \theta - \theta_{eva}\right) + W_{eva}\delta\left(r_{eva}, \theta_{eva}\right)\right]$,

$P_f$ is the fuel porosity, $K_p$ is the permeability coefficient, m$^2$; $s$ is the size of a pore, m; $\mu$ is the coefficient of dynamic viscosity, Pa·s; $\beta$ is the compressibility factor of gaseous pyrolysis products, 1/Pa; $f_i$ is a function describing a change in the mass flow rate of a mixture of water vapor and pyrolysis gases due to the release of volatiles and water vapor absorption during its thermochemical interaction with carbon, kg/(m$^3$·s). The vapor filtration rate was determined from the differential expression of the Darcy law in the radial and azimuthal directions, respectively:

$$U_s = -\frac{K_p}{\mu}\frac{\partial p}{\partial r}, \tag{5}$$

$$V_s = -\frac{K_p}{\mu}\frac{1}{r}\frac{\partial p}{\partial\theta}. \tag{6}$$

Temperature distribution in the gas layer around a particle is described by the energy equation. It takes into account the exothermic effects of reactions of main combustible component oxidation by air:

$$C_g\rho_g\frac{\partial T}{\partial t} + C_g\rho_g\omega(r)\frac{\partial T}{\partial r} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\lambda_g\frac{\partial T}{\partial r}\right) + \frac{1}{r\cdot\sin\theta}\frac{\partial}{\partial\theta}\left(\frac{\sin\theta}{r}\lambda_g\frac{\partial T}{\partial\theta}\right) + \sum_{i=1}^3 Q_i W_i, \tag{7}$$

where $\displaystyle\sum_{i=1}^3 Q_i W_i = Q_{CH_4+O_2} W_{CH_4+O_2} + Q_{CO+O_2} W_{CO+O_2} + Q_{H_2+O_2} W_{H_2+O_2}$, $C_g$ and $\rho_g$ are the heat capacity and the density of gas mixture, $Q_i$ and $W_i$ are the thermal effect and the rate of chemical reaction of fuel oxidation, $\omega(r)$ is the velocity of vapor-gas mixture (m/s). The latter was calculated by formula [30]:

$$\omega(r) = U_s(r_{out}, \theta, t)\cdot\frac{0.96}{0.07\, r/s + 0.29}. \tag{8}$$

At the interface of the "CWF particle – gas medium" system, the boundary condition of the 4th kind was accepted. The exothermic effect of carbon reaction with atmospheric oxygen

(by analogy with [31]) and the thermal radiation of external environment [32] were taken into account:

$$\frac{\partial T}{\partial r} = K_\lambda \frac{\partial T}{\partial r} + \frac{\varepsilon \cdot \sigma \cdot \left(T_g^4 - T\big|_{r=r_0}^4\right) + Q_{C+O_2} \cdot W_{C+O_2}}{\lambda_{cwf}}, \tag{9}$$

$$T\left(r_{out}, \theta, t\right)\big|_{r=r_{out}+0} = T\left(r_{out}, \theta, t\right)\big|_{r=r_{out}-0},$$

here, $K_\lambda = \lambda_g / \lambda_{cwf}$, $\varepsilon$ is the integral emissivity, $\sigma$ is the Stefan–Boltzmann constant. The rate of reaction $C + O_2 = CO_2 + 18.67$ MJ/kg was calculated using the mathematical expression of Arrhenius law

$$W_i = k_{C+O_2} \cdot \left[1 - \sum_{i=1}^{n} c_i\left(r_{out}, \theta, t\right)\right] \cdot \eta\left(r_{out}, \theta, t\right) \cdot \rho_g \cdot \exp\left(-\frac{E_{C+O_2}}{RT}\right). \tag{10}$$

When stating the problem it was assumed that steam enters the endothermic chemical interaction with coal: $C + H_2O = CO + H_2 - 118.485$ MJ/kg. The rate of this reaction was calculated from relationship [21]

$$W_{C+H_2O} = k_{C+H_2O} \cdot c_{H_2O} \cdot \rho_s \cdot \exp\left(-\frac{E_i}{RT}\right). \tag{11}$$

It was also assumed that decomposition of fuel with the release of volatiles starts when condition $T_{sur} \geq T_{std}$ is reached on the particle surface ($T_{sur}$ is the temperature of particle surface, $T_{std}$ is the temperature of thermal decomposition beginning). The process of thermal decomposition is described by the equation of chemical kinetics:

$$\frac{\partial \eta}{\partial t} = (1 - \eta) \cdot k_{c \to vol} \cdot \exp\left(-\frac{E_{c \to vol}}{RT}\right), \tag{12}$$

where $\eta$ is the mass fraction of decomposed material, $k$ is the pre-exponential factor (s$^{-1}$), $E$ is the activation energy of thermal decomposition (J/mol). The rate of pyrolysis was calculated by relationship

$$W_i = M^{daf} \cdot (1 - \eta) \cdot k_{c \to vol} \cdot \rho_{wcf} \cdot \exp\left(-\frac{E_{c \to vol}}{RT}\right), \tag{13}$$

where, $M^{daf}$ is the contents of volatiles. The products of thermal decomposition and chemical interaction of a solid residue and water vapors are blown into the near-wall region. A gas mixture, flammable upon reaching the critical values of fuel temperature and concentration, is formed [21]. The chemical compositions of volatiles are given in Table 1. The time period from the beginning of thermal effect on the particle to the beginning of intensive chemical interaction of the vapor-gas mixture with oxidizer is considered the time of ignition delay. The amount of heat released due to fuel oxidation should exceed the amount of heat coming from the heat source (external environment). In the immediate vicinity of the particle surface, three most significant reactions [20] were taken into account:

1. $H_2 + 0.5 O_2 = H_2O + 141900$ kJ/kg,

2. $CO + 0.5 O_2 = CO_2 + 10090$ kJ/kg,

3. $CH_4 + 2 O_2 = 2H_2O + CO_2 + 55000$ kJ/kg.

The rate of these reactions was calculated from the mathematical expression of the Arrhenius law

$$W_i = k_i \, c_i(r, \theta, t) \left( 1 - \sum_{i=1}^{n} c_i(r, \theta, t) \right) \rho_{\mathrm{g}} \exp\left( -\frac{E_i}{RT} \right). \qquad (14)$$

Concentrations of components of the gas-vapor mixture ($H_2$, $CO$, $CH_4$, $CO_2$, and $H_2O$) in the near-wall region were calculated when solving the diffusion equations for the corresponding reaction component:

$$\rho_{\mathrm{g}} \frac{\partial c_i}{\partial t} + \rho_{\mathrm{g}} \, \omega(r) \frac{\partial c_i}{\partial r} = \frac{\rho_{\mathrm{g}}}{r^2} \frac{\partial}{\partial r}\left( r^2 D_i \frac{\partial c_i}{\partial r} \right) + \frac{\rho_{\mathrm{g}}}{r \cdot \sin\theta} \frac{\partial}{\partial \theta}\left( \frac{\sin\theta}{r} D_i \frac{\partial c_i}{\partial \theta} \right) - \sum_{i=1}^{3} W_i, \qquad (15)$$

where $c_i$ are the concentrations of pyrolysis products, $D$ is the diffusion coefficient, $m^2/s$. As is known [33], at thermal decomposition of coal, a destruction accompanied by an increase in pore sizes occurs. Under these conditions, when formulating the problem, a change in the coal density $\rho_3$ and the fuel porosity $P_{\mathrm{f}}$ was taken into account:

$$\frac{\partial \rho}{\partial t} = (\rho - \rho_{\mathrm{etd}}) \cdot k_{\mathrm{w \to vol}} \cdot \exp\left( -\frac{E_{\mathrm{w \to vol}}}{R \cdot T} \right), \qquad (16)$$

$$P_{\mathrm{f}} = P_0 \, (\rho - \rho_0)/(\rho_{\mathrm{etd}} - \rho_0). \qquad (17)$$

The system of equations (1)–(17) was solved under the following initial

$$t = 0 \to \begin{cases} T(r, \theta, 0) = T_0 = 298 \, K, \;\; p(r, \theta, 0) = p_{\mathrm{atm}}, \\ \rho\,(r, \theta, 0) = \rho_0, \;\; \eta(r, \theta, 0) = 0 \\ T(r, \theta, 0) = T_{\mathrm{g}}, \;\; c_i(r, \theta, 0) = 0, \end{cases} \begin{array}{l} 0 < r < r_{\mathrm{out}}, \;\; 0 < \theta < \pi, \\ \\ r_{\mathrm{out}} < r < r_{\mathrm{g}}, \;\; 0 < \theta < \pi, \end{array}$$

and boundary conditions

$$\left.\frac{\partial T}{\partial r}\right|_{\substack{r=0 \\ 0<\theta<\pi}} = 0, \quad \left.\frac{\partial T}{\partial \theta}\right|_{\substack{0<r<r_{\mathrm{g}} \\ \theta=0 \\ \theta=\pi}} = 0, \quad \left.\frac{\partial^2 T}{\partial r^2}\right|_{\substack{r=r_{\mathrm{g}} \\ 0<\theta<\pi}} = 0, \quad \left.\frac{\partial p}{\partial r}\right|_{\substack{r=0 \\ 0<\theta<\pi}} = 0, \quad \left.\frac{\partial p}{\partial \theta}\right|_{\substack{0<r<r_{\mathrm{out}} \\ \theta=0 \\ \theta=\pi}} = 0,$$

$$\qquad (18)$$

$$\left. p \right|_{\substack{r=r_{\mathrm{out}} \\ 0<\theta<\pi}} = p_{\mathrm{atm}}, \quad \left.\frac{\partial c_i}{\partial r}\right|_{\substack{r=r_{\mathrm{out}} \\ 0<\theta<\pi}} = \frac{W_i}{\rho_{\mathrm{g}} D_i}, \quad \left.\frac{\partial^2 c}{\partial r^2}\right|_{\substack{r=r_{\mathrm{g}} \\ 0<\theta<\pi}} = 0, \quad \left.\frac{\partial c}{\partial \theta}\right|_{\substack{0<r<r_{\mathrm{g}} \\ \theta=0 \\ \theta=\pi}} = 0.$$

Heat conductivity, heat capacity and density of wet and "dehydrated" parts of coal-water fuel were calculated taking into account the volume fractions of the components:

$$\lambda_{\mathrm{cwf}} = \begin{cases} \lambda_1, \;\; r \le r_{\mathrm{eva}} \\ \lambda_2, \;\; r > r_{\mathrm{eva}} \end{cases}, \quad C_{\mathrm{cwf}} = \begin{cases} C_1, \;\; r \le r_{\mathrm{eva}} \\ C_2, \;\; r > r_{\mathrm{eva}} \end{cases}, \quad \rho_{\mathrm{cwf}} = \begin{cases} \rho_1, \;\; r \le r_{\mathrm{eva}} \\ \rho_2, \;\; r > r_{\mathrm{eva}} \end{cases},$$

then,

$$\begin{aligned} \lambda_1 &= \varphi_3 \lambda_3 + \varphi_4 \lambda_4, \quad \lambda_2 = \varphi_3 \lambda_3 + \varphi_5 \lambda_5, \\ C_1 &= \varphi_3 C_3 + \varphi_4 C_4, \quad C_2 = \varphi_3 C_3 + \varphi_5 C_5, \\ \rho_1 &= \varphi_3 \rho_3 + \varphi_4 \rho_4, \quad \rho_2 = \varphi_3 \rho_3 + \varphi_5 \rho_5, \end{aligned} \qquad (19)$$

where $\varphi$ is volume fraction of the corresponding fuel component; subscripts: 3 is coal, 4 is water, 5 is water vapor. The thermophysical characteristics of the gas-vapor mixture were also calculated taking into account the volume fractions of the components:

$$\lambda_g = \sum_{i=1}^{n} \varphi_i \lambda_i + \left(1 - \sum_{i=1}^{n} \varphi_i\right) \lambda_g, \quad C_g = \sum_{i=1}^{n} \varphi_i C_i + \left(1 - \sum_{i=1}^{n} \varphi_i\right) \cdot C_g,$$

$$\rho_g = \sum_{i=1}^{n} \varphi_i \rho_i + \left(1 - \sum_{i=1}^{n} \varphi_i\right) \cdot \rho_g. \tag{20}$$

The volume fractions of the components of vapor-gas mixture are calculated from their mass concentrations:

$$\varphi_i = (c_i/\rho_i) \bigg/ \sum_{i=1}^{n} \frac{c_i}{\rho_i}. \tag{21}$$

### Initial data

Ignition of particles of coal-water fuel made of coal and brown coal was studied. Their thermophysical and thermochemical characteristics are given in Table 2. As was mentioned earlier, coal heating leads to thermal decomposition of the organic part of fuel and it is accompanied by the release of volatiles. The composition of the latter is given in Table 1. Thermochemical constants of pyrolysis, steam gasification, and ignition reactions are given in Table 3. Numerical studies were carried out for the following initial data: $T_0 = T(r, \theta, t) = 298$ K, $p_a = 101325$ Pa, $\eta_0 = 0$, $M_{wat} = 0.018$ kg/mol, $K_p = 10^{-11}$ m$^2$.

### Method of solving equations

The formulated initial- and boundary-value problem was solved by the finite-difference method [41, 42]. System (1)–(17) was implemented during a time period until the conditions adequate to ignition of solid, liquid, and heterogeneous fuels were reached [16]. To determine the point in time corresponding to the ignition of the gas mixture, we used the criterion introduced into the ignition theory by D.A. Frank-Kamenetskiy [43], namely: "The heat released by a chemical reaction in its zone exceeds the heat supplied by the external environment to this zone due to heat conduction, radiation, and convection".

It should be noted that the calculations of the processes of fuel ignition in the presence of intense phase transformations (in particular, evaporation) are among the most complex in the theory of combustion. This relates to the fact that the evaporation of water proceeds

**Table 2**

**Thermophysical and thermochemical characteristics of coals [26, 34, 35]**

| Coals of Donetsk coal basin | | | | | | |
|---|---|---|---|---|---|---|
| Coal grade (deposit) | $C_p$, J/(kg·K) | $Q_{c\rightarrow vol}$, J/kg | $\lambda$, W/(m·K) | $\rho$, kg/m$^3$ | $M^{daf}$, % | $C^{pcm}$, % |
| Long-flame | 1150 | 176.7 | 0.116 | 1253 | 46 | 76 |
| Gas | 1130 | 193.8 | 0.123 | 1264 | 39 | 83 |
| Fat | 1090 | 282.6 | 0.119 | 1260 | 26 | 86 |
| Coke | 1070 | 287.2 | 0.128 | 1254 | 28 | 88 |
| Lean sintering | 1050 | 296.4 | 0.134 | 1274 | 33 | 89 |
| Lean | 1000 | 274.2 | 0.134 | 1242 | 15 | 90 |
| Semi-anthracite | 946 | 193 | 0.149 | 1307 | 9 | 91 |
| Anthracite | 928 | 187.6 | 0.149 | 1389 | 1.5 | 95 |
| Brown coal | | | | | | |
| Coal grade (deposit) | $C_p$, J/(kg·K) | $Q_{c\rightarrow vol}$, J/kg | $\lambda$, W/(m·K) | $\rho$, kg/m$^3$ | $M^{daf}$, % | $C^{pcm}$, % |
| Berezovskoe | 1150 | 431 | 0.151 | 1200 | 48 | 34.3 |
| Gusinoozerskoe | 1140 | 451 | 0.140 | 1200 | 43 | 39.4 |
| Novo-Dmitrovskoe | 1130 | 196 | 0.151 | 1200 | 43 | 44.4 |
| Irsha-Borodinskoe | 1170 | 490 | 0.140 | 120 | 47 | 37 |

**T a b l e  3**

**Constants of thermochemical reactions**

| Reaction | $E_i$, J/(mol) | $k_i$, 1/s | Works |
|---|---|---|---|
| Thermal decomposition c→vol | $31.0 \cdot 10^3$ | 24 — brown coal | [36] |
| | $56.1 \cdot 10^3$ | 178 — fat coal | |
| | $56.9 \cdot 10^3$ | 131.8 — coke | |
| | $60.6 \cdot 10^3$ | 212 — lean coal | |
| $H_2O+C = CO+H_2$ | $220 \cdot 10^3$ | $2.07 \cdot 10^7$ | [37] |
| $CO+O_2 = CO_2$ | $200.0 \cdot 10^3$ | $2.50 \cdot 10^{12}$ | [38] |
| $H_2+0.5 \cdot O_2 = H_2O$ | $105.0 \cdot 10^3$ | $1.13 \cdot 10^{17}$ | [39] |
| $CH_4+O_2 = CO_2+2 \cdot H_2O$ | $35 \cdot 10^3$ | $5.1 \cdot 10^{14}$ | [40] |

in a very narrow (much smaller than the linear size of a particle) region: evaporation front. As a rule, the thermal effects of phase transitions are very high (up to $2.5 \cdot 10^6$ J/kg). As a result, internal local heat sink occurs in a wet particle. The numerical study is complicated by the fact that the time scales of evaporation and ignition processes differ significantly: ignition is a fast process, and evaporation is much slower. For this reason, to solve the problem, a special algorithm based on the solution of the problem of water evaporation by the method of implicit separation of phase transition front was developed [44].

### Results and discussion

Times of ignition delay are presented in Fig. 2 for coal-water fuel droplets made of various types of coals (see Table 1): long-flame, gas, fat, coke, lean sintering, lean, semi-anthracite, and anthracite. To verify the mathematical model, the figure shows the experimental [19] values of ignition delay ($t_{ign}$) of CWF particles based on long-flame coal. It can be noted that theoretical and experimental ignition delay times are reliably consistent (within a confidence interval of ±17 %).

The analysis of dependences shows that under the conditions of relatively high temperatures ($T_g \geq 1073$ K), the ignition delay times for CWF particles made of black coal of various grades differ slightly (not more than by 10 %). Simultaneously, at low temperatures of external environment ($T_g \approx 1073$ K), the values of $t_{ign}$ for CWF based on coal differ significantly. Obviously, this indicates that thermophysical processes (inert heating due to radiation and convection, evaporation of water), which occur at the stage of thermal preparation, but not the ignition
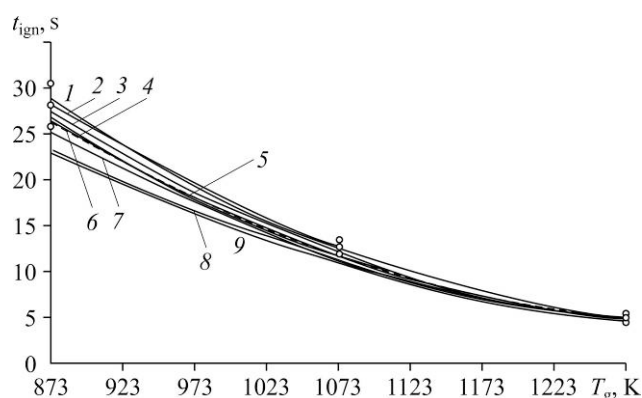


*Fig. 2.* Times of ignition delay for the particles of coal-water fuel made of various grade coals vs. temperature of external environment.

Coal grades: *1* — fat coal, *2* — long-flame coal, *3* — coke, *4* — gas coal, *5* — long-flame coal, *6* — lean sintering coal, *7* — lean coal, *8* — semi-anthracite, *9* — anthracite;
*2* — experiment [20], *1*, *3–9* — numerical solution to system (1)–(33); size of CWF particles — $3 \cdot 10^{-3}$ m.

kinetics, play the decisive role when igniting the CWF drops. Most likely, duration of the ignition period is determined by combination of thermophysical (thermal conductivity ($\lambda$), heat capacity ($C$), density ($\rho$)) and thermochemical (heat of thermal decomposition) properties.

The analysis of dependences shows that anthracite and semi-anthracite based CWF particles ignite faster than others in almost the entire range of ambient temperatures. This is due to the low value of heat capacity of fuel and high carbon content. The ignition of CWF particles made of fat coal is the slowest. The latter is associated with higher values of heat capacity and heat of thermal decomposition of basic fuel.

The delay times for ignition of a CWF particle based on brown coal are shown in Fig. 3 depending on the ambient temperature. To verify the mathematical model, a comparative analysis of experimental and theoretical values of $t_{ign}$ is presented in a graphical form. It showed their reliable matching. According to the analysis of these dependencies, it can be noted that ignition of fuel particles prepared from coal of Novo-Dmitrovskoye deposit are the fastest. This is explained, firstly, by low values of base fuel heat capacity and heat of thermal decomposition in comparison with other coals, and secondly, by the content of sufficiently large amount of volatiles and carbon in the coal structure of Novo-Dmitrovskoye deposit.

Comparison of dependences $t_{ign}(T)$ in Figs. 2 and 3 shows that combustion of coal-water fuel droplets based on brown coal starts much faster than combustion of coal-based particles. This is caused, primarily, by a higher volatile content in brown coal. Results of comparative analysis of ignition delay times obtained numerically and experimentally in [20] showed their satisfactory agreement.

Time dependences of surface temperature $T_{sur}$ of CWF particles made of coal of various grades are shown in Fig. 4. The ambient temperature is $T_g = 1273$ K. Analysis of dependences $T_{sur} = f(t)$ shows that the entire induction period can be divided into a series of successive stages: inert heating, dewatering of coal-water particle, ignition. The initial period of time (inert radiation-convective heating) is not more than 18 % of $t_{ign}$ and it is characterized by a rapid increase in temperature. After this, the process of intensive evaporation of water is initiated. As a result, a highly porous carbon frame with low heat conductivity and heat capacity is formed in the particle. At the same time, the temperature rise slows down. The latter is caused by a decrease in the radiation heat flux from the external environment to the fuel particle. It can
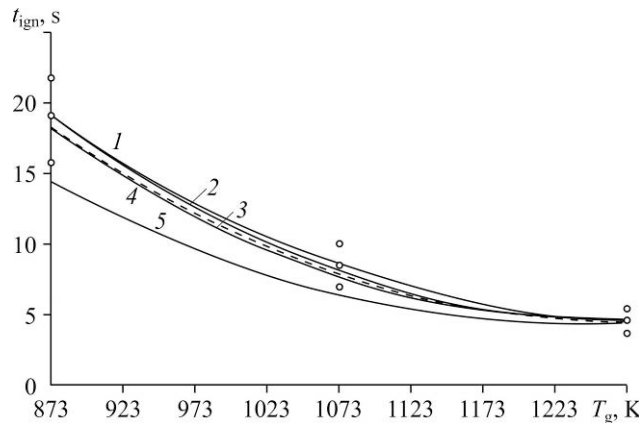


*Fig. 3.* Times of ignition delay for the particles of coal-water fuel made of brown coals vs. temperature.

*1* — Berezovskoe deposit, *2* — Irsha-Borodinskoe coal, *3* — Berezovskoe deposit,
*4* — Gusinoozersk deposit, *5* — Novo-Dmitrovskoe deposit;
*1* — experiment [20], *2–5* — numerical solution to system (1)–(21).

be noted that the period of water removal from the particle is up to 70 % of the total ignition time. This is most likely due to the high endothermic effect of the phase transition (up to 2.5 MJ/kg), which causes a slowdown in the growth rate of $T_{sur}$. In Fig. 4, we can note the characteristic bend of $T_{sur}(t)$ curve at time $t \approx 0.9 \cdot t_{ign}$, which corresponds to the moment of ignition. Curve $T_{sur}(t)$ takes exponential character: $\partial T/\partial t \approx \exp(-E/(RT))$.

Time diagrams of variation of the surface temperature of CWF particles made of brown coal at ambient temperature $T_g$ = 1273 K are presented in Fig. 5. According to the results of analysis, we can make a conclusion similar to the conclusion in Fig. 4. It should be noted that the surface temperature of CWF particles made of brown coal from the Novo-Dmitrovskoe deposit grows much faster than that of other fuels. As was noted, this is due to low heat capacity and thermal effect of thermal decomposition. The results shown in Figs. 4 and 5 correlate completely with the data of [16–20] as well as with the dependences obtained in [45] and [46].

Temperature distributions (in dimensionless form) in the "coal-water particle – gas environment" system at the time of ignition of volatiles from CWF droplets made of coal are shown in Fig. 6. It can be noted that the ignition zone of gaseous pyrolysis products is located at some distance (approximately, at a half diameter of a CWF drop) from the surface of the particle. The location of the ignition zone does not depend on the type of basic fuel and, accordingly, on the volatile content. It can be reasonably assumed that the mechanism of combustion initiation is significantly affected by convection of pyrolysis products and water vapors. In this case, the use of the infinitely thin "film" method (by analogy with [36]) in the ignition zones of coal-water fuels is not sufficiently substantiated. We should also note that ignition of volatiles can occur even before complete evaporation of interstitial moisture of fuel.

Distributions of dimensionless temperatures in the "CWF particle-gas medium" system at gas-phase ignition of a coal-water fuel droplet based on brown coal are shown in Fig. 7 for ambient temperature $T_g$ = 1273 K. Analysis of dependences in Fig. 7 allows a conclusion similar to that made for Fig. 6.
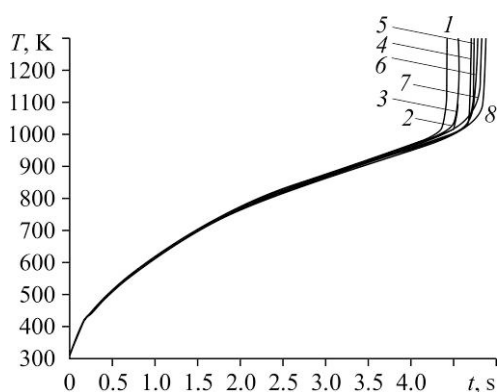
*Fig. 4.* Dependence of surface temperature of a coal-water fuel particle (made of various grade coals) on time.

*1* — semi-anthracite, *2* — anthracite, *3* — lean coal, *4* — lean sintering coal, *5* — coke, *6* — gas coal, *7* — long-flame coal, *8* — fat coal.
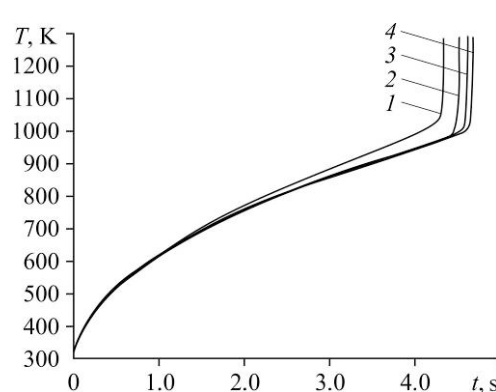
*Fig. 5.* Dependence of surface temperature of a coal-water fuel particle (based on brown coal) on time.

*1* — Novo-Dmitrovskoe deposit, *2* — Berezovsky deposit, *3* — Gusinoozerskoe deposit, *4* — Irsha-Borodinskoe deposit.
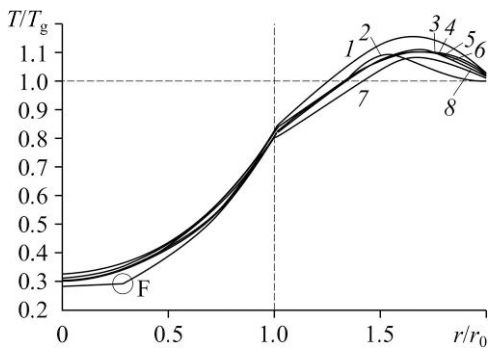
*Fig. 6.* Temperature distribution in "CWF particle – high-temperature medium" system at the moment of ignition of fuel drops based on coal.
Temperature of the external medium $T_g$ = 1273 K;
*1* — fat, *2* — anthracite, *3* — semi-anthracite, *4* — lean coal, *5* — lean sintering coal, *6* — coke, *7* — long-flame coal, *8* — gas coal;
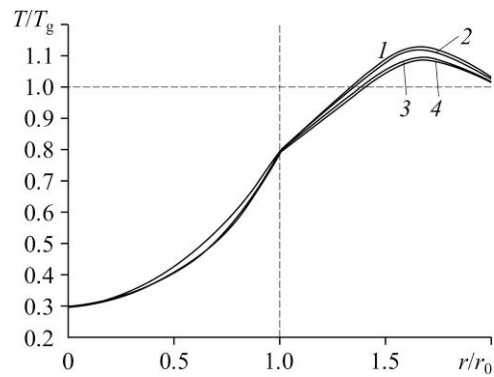F — evaporation front.



*Fig. 7.* Temperature distribution in "CWF particle – high-temperature medium" system at the moment of ignition of fuel drops based on brown coal.
*1* — Gusinoozerskoe deposit,
*2* — Irsha-Borodinskoe deposit,
*3* — Novo-Dmitrovskoe deposit,
*4* — Berezovskoe deposit.

Analysis of publications on the problem presented has shown that there are no experimental data on times of ignition delay of coke residue. For this reason, only parametric analysis of the process of carbon combustion initiation was carried out. The times of coke ignition delay are presented in Fig. 8. According to analysis of $t_{ign}(T_g)$, coke begins burning almost immediately after ignition of volatiles. The interval between the times of ignition of volatiles and coke does not exceed 0.5 seconds. Such a tendency is kept for the particles of CWF made of both black and brown coal. The nature of dependencies in Fig. 8 shows that the degree of coal metamorphism has a significant impact on characteristics and conditions of ignition. Thus, under the conditions of relatively low ambient temperatures ($T_g$ <1173 K), brown coal-based CWF droplets ignite much faster (by about 50 %) than coal-based fuels. This is due to the high content of volatiles. Under the conditions of high temperatures ($T_g$ ≥1273 K), the difference in
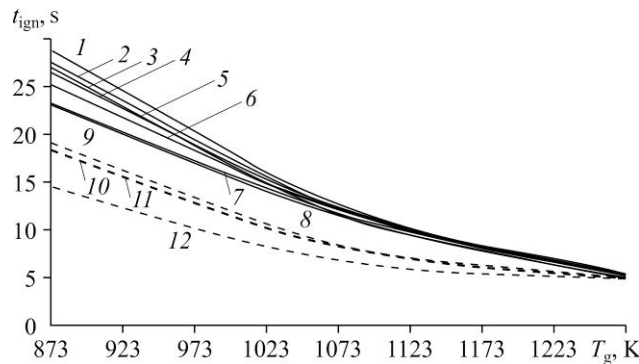


*Fig. 8.* Dependence of delay time of ignition of coal-water fuel particles (of size $3 \cdot 10^{-3}$ m), made of various grade coals on the temperature of external environment.
Coals: *1* — fat coal, *2* — coke, *3* — gas coal, *4* — long-flame coal, *5* — lean sintering coal, *6* — lean coal, *7* — semi-anthracite, *8* — anthracite;
brown coals: *9* — Irsha–Borodinskoe coal, *10* — Gusinoozerskoe deposit, *11* — Berezovsky deposit, *12* — Novo–Dmitrovskoe deposit;
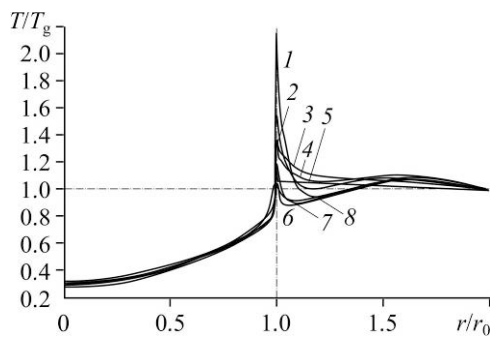
*Fig. 9.* Temperature distribution in "CWF particle – high-temperature medium" system at the moment of fuel coke ignition.

Coal-water fuel based on coals of different grades:
*1* — lean sintering coal, *2* — fat coal,
*3* — semi-anthracite, *4* — lean coal,
*5* — anthracite, *6* — coke, *7* — flame coal,
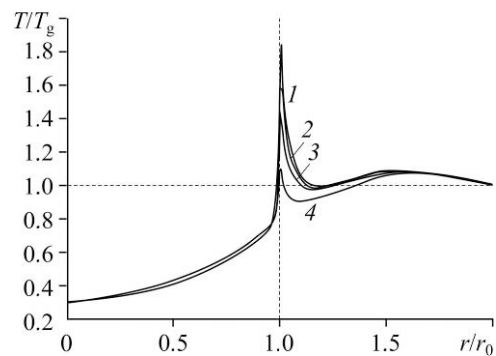*8* — gas coal.

*Fig. 10.* Temperature distribution in "CWF particle – high-temperature medium" system at the moment of ignition of fuel drops based on brown coal.

*1* — Gusinoozerskoe deposit,
*2* — Irsha-Borodinsky coal, *3* — Berezovsky deposit,
*4* — Novo-Dmitrovskoe deposit.

times of ignition delay for brown coal and black coal CWF drops is insignificant. This is probably explained by the fact that at high values of $T_g$, dynamics of the ignition process is controlled not only by the ignition kinetics, but also by thermophysical processes occurring during the period of thermal preparation.

Temperature distribution in the "coal-water particle – gas medium" system at the ignition of coke residue is shown in Fig. 9 for ambient temperature $T_g = 1273$ K. At the time of coke ignition, the temperature at the particle center is at least 373 K. Accordingly, it can be argued that the coke of a fuel particle can be ignited only after its complete dehydration. An exception is the process of igniting the CWF droplets based on long-flame coal. It can be stated that oxidation of such fuel under the conditions of continuing evaporation will differ significantly from dry coal burning.

Temperature distribution in the "coal-water particle – high-temperature environment" system at ignition of fuel made of brown coal is shown in Fig. 10 for ambient temperature $T_g = 1273$ K. Analysis of dependencies allows a conclusion similar to that made for Fig. 9 that coke of coal-water particles ignites after dehydration of the main layer of fuel. This correlates with theoretical results of [16–18].

### Conclusions

A new mathematical model of the process of coal-water particle ignition was developed. This model takes into account a degree of coal metamorphism and combination of the main processes of heat and mass transfer under the conditions of intense phase and thermochemical transformations at thermal preparation. According to the simulation results, the integral characteristics of the process of ignition of coal-water fuel droplets made of black and brown coals of various grades were determined. Comparative analysis of the ignition delay times obtained theoretically and experimentally [20] revealed their reliable correspondence.

It is shown that the type and grade of coal can have a significant effect on characteristics and conditions of ignition. It has been determined that coal-water particles made of anthracite and semi-anthracite ignite faster (by about 20 %) than the CWF drops prepared of other coals.

Ignition of fat-coal CWF drops is the slowest. This is primarily due to a lower heat capacity and higher heat conductivity of anthracite and semi-anthracite coals in comparison with fat coal as well as the relatively low thermal effect of thermal decomposition of fuel.

Under conditions of relatively low ambient temperatures ($T_g$ <1173 K), brown coal-based CWF droplets ignite much faster (by about 50%) than coal-based fuels. This is because of the high content of volatiles in the brown coal. It should be noted that under the conditions of high temperatures ($T_g \geq$ 1273 K), the difference in the ignition delay times for brown-coal and black-coal CWF drops is insignificant. Thus, it can be reasonably concluded that the duration of the period of coal-water fuel induction is determined not only by the kinetics of ignition, but also by thermal processes occurring during the period of thermal preparation.

## *Nomenclature*

$T$ — temperature, K,
$\sigma$ — Stefan–Boltzmann constant, W/(m$^2$·K$^4$),
$\alpha$ — absorption coefficient, 1/m,
$\varepsilon$ — integral emissivity coefficient,
$p$ — pressure, Pa,
$\eta$ — degree of fuel pyrolysis,
$k$ — pre-exponential factor for heterogeneous (m/s) or homogeneous (1/s) reaction,
$U$ — radial velocity of water vapor motion, m/s,
$V$ — azimuthal velocity of water vapor motion, m/s,
$M$ — contents of volatiles,
$M_{wat}$ — molar mass of water, kg/mol,
$E$ — activation energy of thermal decomposition, J/mol,

$P_f$ — fuel porosity,
$K_p$ — coefficient of coal permeability, m$^2$,
$\mu$ — dynamic viscosity, Pa·s,
$Q$ — thermal effect, J/kg,
$W$ — mass rate of chemical reaction, kg/m$^2$/s,
$\lambda$ — coefficient of heat conductivity, W/(m·K),
$C$ — heat capacity, J/(kg·K),
$c$ — concentration,
$\rho$ — density, kg/m$^3$,
$r$ — radius, m,
$h_{spr}$ — parameter of evaporation front spreading, m,
$s$ — characteristic size of pore, m,
$t$ — time, s.

## *Indices*

0 — initial time,
1 — area of initial fuel,
2 — area of dry fuel,
3 — coal,
4 — water,
5 — water vapors,
f — fuel,
F — evaporation front,
g — high-temperature gas,
c — coke residue,
$i$ — reaction number,
s — steam,
a — ambient,

fp — water freezing point,
eva — "wet fuel – dry carbon frame" interface,
ign — ignition,
out — outer radius of particle,
std — beginning of thermal decomposition process,
etd — end of thermal decomposition process,
sur — particle surface,
c→vol — process of thermal decomposition,
cwf — coal-water suspension,
wat — water,
daf — dry ash-free fuel,
vol — volatiles,
pcm — per combustible mass.

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