Heat and mass transfer in a coal-water fuel particle at the stage of "thermal" treatment[*]

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The problem of heat and mass transfer has been solved numerically under the conditions of coal-water fuel particle ignition. The concurrent processes of evaporation, filtration of steam, thermal decomposition of the organic part of coal, thermal and chemical interaction of steam and coke carbon, and oxidation of products of their reaction and volatiles by the external oxidizer have been taken into account. The scales of influence of individual thermophysical and thermochemical properties of coals on the characteristics and conditions of ignition of coal-water slurry have been determined.

Key words: convective-radiative heat transfer, evaporation, filtration, pyrolysis, ignition, coal-water fuel (CWF).

Introduction

The possible usage of coal-water fuels (CWF) as a major fuel in the furnaces of boiler units of different purpose was substantiated quite long ago [1−3]. The technologies of preparation [4], transportation [5], and combustion [6] of such fuels were developed; and the design solutions for the methods and technical devices for various stages of the technological cycle from grinding of the source natural fuel to combustion were proposed [7−10]. However, to date there have been no examples of sustainable use of these technologies in Russia. Most likely, the latter is not only due to underdevelopment of the technical or technological aspects of the CWF application, but also to the lack of scientific knowledge on a number of scientific and technical problems, such as coal grinding to ultrafine state, thermal preparation, ignition and combustion of the fuel particles.

One of the most difficult is the problem of determining the conditions and characteristics of ignition of the coal-water fuel particles in the range of parameters corresponding to the furnace of a typical boiler unit. The modern theory of ignition of solid fuels (including coals) [11−13] cannot be formally applied to describe the processes of heat transfer in CWF particles due to a large (as shown by the results of [14−16]) role of local phase transformations (evaporation of water in this case) in the formation of the temperature field of the heated layer of the condensed substance in the period that precedes ignition. Certain, and in many cases, rather significant influence on the conditions and characteristics of ignition may be exerted by

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individual properties of CWF: thermophysical properties, ash content, percentage of volatile components, and kinetics of thermal decomposition of the organic part of fuel, etc.

A mathematical model describing the main physical-chemical processes and heat and mass transfer in the CWF particle during "thermal preparation" was developed in [17, 18]. The model [17, 18] differs from the known ones [19–20] by a more detailed analysis of the processes of heat and mass transfer. However, the results of theoretical studies [17, 18] are insufficient for conclusions about variability of the used model of heat and mass transfer in CWF in terms of intense heating, describing the conditions of ignition of particles of the CWF slurry with different bases.

The aim of this work is to analyze the conditions and characteristics of ignition of particles of the group of coal-water fuels, using a model that takes into account the main processes of heat and mass transfer occurring in the CWF particle under intense heating.

Problem statement

The statement of the problem of heat and mass transfer in a spherical particle of coal-water fuel was focused on the description of the complex interrelated processes of physical and chemical transformation. The most important for forming the temperature field and, consequently, for determining the intensity of gasification of the organic part of coal are the processes of water evaporation, thermal decomposition of coal, and chemical interaction of gaseous and solid products of pyrolysis with steam and external oxidizers. It should be noted that the phase transition at the "water–vapor" boundary with the most significant contribution in the heat balance of the CWF particle is the most complicated for mathematical description. The solution of Stefan problem (similar to [19]) requires knowledge of the interfacial temperature, for example, at melting or crystallization. However, the motion of the evaporation front in the CWF particle is possible not only at the boiling point, but also at different temperatures of the phase transition surface depending on fuel heating intensity. Therefore, in the problem statement, we used the model of evaporation well-proven in solving problems of liquid fuel ignition at intense evaporation [14–16]. In addition to these physical and chemical processes, we took into account heat transfer by heat conduction, filtration of steam and products of gasification of the organic part of fuel. Convective and radiative heat transfer between CWF particles and external medium was also considered.

By analogy with the formulation of the problem [17], the system of equations describing heat transfer and high-temperature physical-chemical conversion on the surface of the CWF particle can be formulated in the form:

– the energy equation for the source part of the fuel:

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

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

– the energy equation for the "dry" part of CWF:

$$C_2 \rho_2 \frac{\partial T_2(r,t)}{\partial t} = \frac{1}{r^2} \cdot \frac{\partial}{\partial r} \left[r^2 \cdot \lambda_2 \cdot \frac{\partial T_2(r,t)}{\partial r} \right] - \sum Q_i \cdot W_i - u \, C_p \cdot \rho \frac{\partial T_2(r,T)}{\partial r}, \tag{2}$$

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

where T_v is the temperature at the boundary of vaporization, K; Q_i is the thermal effect of chemical reaction, J/kg; W_i is the chemical reaction rate, kg/(m²·c); u is the rate of steam filtration, m/s; λ_1 is the coefficient of thermal conductivity of the source part of CWF, W/(m·K); λ_2 is the coefficient of thermal conductivity of the dry part of CWF, W/(m·K); C_1 is the heat capacity of the source part of CWF, J/(kg·K); C_2 is the heat capacity of the dry part of the CWF, J/(kg·K); ρ_1 is the density of the source part of CWF, kg/m³; ρ_2 is the density

of the dry part of CWF, kg/m^3; C_p is the isobaric heat capacity of steam, J/(kg·K); ρ is the vapor density, kg/m^3; r_v is the radius of the evaporation front, m; and r_0 is the outer radius of the particle, m.

The problem statement assumed that evaporation of water occurs at the interface of the system "the source CWF – a dry coal". Accordingly, when $r = r_v$, the boundary condition of the 4th kind considering the thermal effect of phase transition is satisfied:

$$\lambda_1 \frac{\partial T_1(r,t)}{\partial r}\bigg|_{r=r_v-0} - \lambda_2 \frac{\partial T_2(r,t)}{\partial r}\bigg|_{r=r_v+0} = Q_v \cdot W_v, \tag{3}$$

$$T_1(r_v, t) = T_2(r_v, t) = T_v.$$

The mass rate of water evaporation (W_v, kg/(m^2·s)) was calculated from the expression [16]:

$$W_v = W_0 \cdot \exp\left(\frac{Q_v \cdot \mu \cdot (T_v - T_{frz})}{R \cdot T_0 \cdot T_v}\right), \tag{4}$$

where T_{frz} is the water temperature corresponding to the freezing point, K; μ is the molar mass of steam, kg/mol; R is the universal gas constant, J/(mol·K); W_0 is the mass rate of water evaporation at the temperature T_{frz}, kg/(m^2·s); and Q_v is the thermal effect of water evaporation, J/kg.

The coordinate of evaporation boundaries was found from the expression:

$$r_f = r_0 - \int_0^\tau u_f d\tau, \tag{5}$$

where $u_f = W_v/\rho_w$ is the linear velocity of evaporation front advancement, m/s.

The filtration of the evaporated moisture through a porous carbon frame and appropriate cooling of the latter one were taken into account. The pressure distribution along the particle radius was calculated using the equation of filtration [17]:

$$\frac{m \cdot v \cdot Z}{K_p} \cdot \frac{\partial p_s(r,t)}{\partial t} = \left(\frac{\partial p_s^2(r,t)}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial p_s(r,t)}{\partial r}\right), \tag{6}$$

$$t > 0, \quad r_v < r < r_0.$$

The vapor filtration rate was calculated using a mathematical expression of Darcy's law:

$$u = -\frac{K_p}{v} \cdot \frac{\partial p_s}{\partial r}, \tag{7}$$

where p_s is the pressure of the steam phase, Pa; m is the porosity; Z is the degree of steam compressibility, 1/Pa; K_p is the permeability of the porous structure, m^2; and v is the dynamic viscosity of steam, Pa·s.

In the problem statement, it was assumed that steam enters in an endothermic chemical reaction with coal remaining after the completion of dehumidification. The rate of the reaction $C + H_2O = CO + H_2 - 118.485$ MJ was calculated from the expression [18]:

$$W_i = k_i \cdot c_i \cdot \rho_s \cdot \exp\left(-\frac{E}{R \cdot T(r,t)}\right), \tag{8}$$

where k_i is the pre-exponent of appropriate reaction, 1/s, c_i is the concentration of the respective component of the chemical reaction, E is the activation energy, J/mol·K; and i is the number of the chemical reaction.

The decomposition of the organic part of the fuel with the release of volatiles in he particle was considered when reaching the condition $T_s \geq T_{tds}$, on the surface, where T_s is the surface temperature, and T_{tds} is the temperature of thermal decomposition start. The process was described by the equation of chemical kinetics:

$$\frac{\partial \eta_2(r,t)}{\partial t} = \left(1 - \eta_2(r,t)\right) \cdot k_i \cdot \exp\left(-\frac{E}{R \cdot T_2(r,t)}\right), \tag{9}$$

$$t > 0, \quad r_{ev} < r < r_0, \quad T \geq T_{fc},$$

where r_{ev} is the radius of the evaporation front, and T_{fc} is the temperature at the interface of the "source CWF – dry coal" system.

The speed of pyrolysis was calculated using the following equation [19]:

$$W_i = \left(1 - \eta(r,t)\right) \cdot k_i \cdot \rho_2 \cdot \exp\left(-\frac{E}{R \cdot T(r,t)}\right), \tag{10}$$

where $\eta(r, t)$ is the parameter of burnout.

In problem solving, it was considered that products of thermal decomposition and chemical interaction of the carbon solid residue and steam were blown into the "wall" area. This formed a gas mixture ignited when reaching the critical values of temperature and concentration. The time period from the beginning of the thermal influence on the particle prior to the intensive (at the advent of flame) chemical interaction of gas-vapor mixture with an oxidizing agent was taken as the ignition delay time. In the vicinity of the surface of the particle, the following reactions were taken into account:

$$1. \ H_2 + 0.5 \cdot O_2 = H_2O + 141900 \text{ kJ/kg};$$

$$2. \ CO + 0.5 \cdot O_2 = CO_2 + 10090 \text{ kJ/kg};$$

$$3. \ CH_4 + O_2 = CO_2 + H_2O + 55546 \text{ kJ/kg}.$$

The rate of these reactions was calculated from the mathematical expression of Arrhenius law [19]:

$$W_i = k_i \cdot c_i \cdot \rho_i \cdot \exp\left(-E/\left(R \cdot T(r,t)\right)\right). \tag{11}$$

The system of equations (1)–(11) was solved under the following boundary conditions and closing relations: $0 < r < r_0$, $T(r,0) = T_0$, $p(r,0) = p_0$, $\eta(r,0) = \eta_0$,

$$-\lambda_2 \frac{\partial T_2(r_0,t)}{\partial r} = \alpha \cdot [T_c - T_2(r_0,t)] + \varepsilon \cdot \sigma \cdot [T_c^4 - T_2^4(r_0,t)] + \sum_i Q_i \cdot W_i, \tag{12}$$

$$\partial T_1(0,t)/\partial r = 0, \tag{13}$$

$$\partial p_s(r_{ev},t)/\partial r = -(v/K_P)u_s(r_{ev},t), \tag{14}$$

$$p(r_0, t) = p_0, \tag{15}$$

here: T_0 is the initial particle temperature, K; T_{am} is the temperature of the ambient medium, K, σ is the constant of blackbody radiation, W/(m²·K⁴), α is the coefficient of convection heat transfer, W/(m²·K), p_0 is the initial pressure, Pa; η_0 is the initial value of burnout parameter; and complex $(\Sigma Q_i \cdot W_i)$ is the thermal effect of reactions taking place in the vicinity of the particle surface, W/m².

The boundary-value problem (1)–(15) was solved in a period of time before reaching the conditions of CWF ignition on the particle surface, adequate to the conditions of solid fuel ignition at local heating [21] and combustible liquid condensed substances [14, 15].

The formulated problem of mathematical physics was solved by the finite difference method. In connection with nonlinear dependences of the rates of phase transformations and thermo-chemical interaction of components, we used the iterative algorithm developed for solving problems of ignition under the conditions of intensive physical and chemical and phase transformations [22] as well as at high-temperature local thermal effect on the condensed substance [23, 24]. The problem of evaporation was solved by the method of successive accumulation of time step [25]. The reliability of the results of simulation was justified by checking the energy balance in the system similar to [26]. The research was conducted at the following initial data: $T_0(r, t) = 293$ K, $\rho_0 = 101325$ Pa, and $\eta_0 = 0$. Thermal characteristics of coals [27, 28] are given in the table.

The thermal conductivity, heat capacity and density of the moist and "dehydrated" parts of the fuel were calculated taking into account volume fractions of components:

$$\lambda_1 = \varphi_3\lambda_3 + \varphi_4\lambda_4, \quad \lambda_2 = \varphi_4\lambda_4 + \varphi_5\lambda_5,$$

$$C_1 = \varphi_3\lambda_3 + \varphi_4\lambda_4, \quad C_2 = \varphi_4 + \varphi_5\lambda_5,$$

$$\rho_1 = \varphi_3\rho_3 + \varphi_4\lambda_4, \quad \rho_2 = \varphi_4 + \varphi_5\lambda_5,$$

where φ is the volume fraction of the respective component of the fuel; the subscript 3 is the water, 4 is the coal, and 5 is the steam.

In the preparation of coal-water fuel it is possible to use suspensions with different coal concentration. The latter can vary in a fairly wide range (from 50 to 80 %), and the mass fraction of water is from 50 to 20 %, respectively. As a rule, the content of additives and plasticizers does not exceed 1% wt. [1–4]. Accordingly, their influence on the characteristics and conditions of ignition is negligible.

The aim of the numerical analysis of the studied process in the framework of the developed model of heat and mass transfer and chemical reaction was to determine the influence of coal properties (depending on the mark and deposit) on the characteristics and conditions of ignition of the coal-water fuel particles.

Results

Coals from three deposits were chosen as basic components of CWF: anthracite (A) of the Donetsk coal basin [27, 28], the coal of grade "D" of the Kuznetsk coal basin, and brown coal of "B-2" grade from Berezovsk Deposit [27, 28]. The numerical simulation has resulted in finding the dependences of ignition delay time (Fig. 1) of CWF particles with typical sizes made from coals of these three frequently used grades. It is worth noting the smallest values of t_i of CWF particles based on brown coal throughout the range of the ambient temperature changes. This regularity is explained by higher reactivity of coals of grade "B-2" due to the high volatile content and low conductivity compared to anthracite [28].

Table

Thermal characteristics of the studied coals [28, 29]

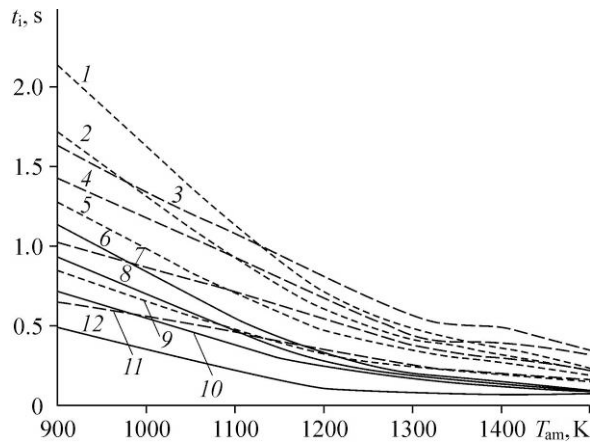| Grade of coal	Thermal conductivity λ_4, W/(m·K)	Heat capacity C_4, kJ/(kg·K)
Donetsk anthracite	0.149	0.98
Kuznetsk coal grade "D"	0.134	1.38
Berezovsk lignite "B"	0.113	1.15

Fig. 1. Dependence of ignition delay time on the temperature of external medium of CWF particles
with different diameters obtained from coals of various grades.

The diameters of particles:: $1 \cdot 10^{-3}$ (*1, 3, 6*), $0.8 \cdot 10^{-3}$ (*2, 4, 8*), $0.6 \cdot 10^{-3}$ (*5, 7, 10*), $0.4 \cdot 10^{-3}$ (*9, 11, 12*) m;
grades of coal: *1, 2, 5, 9* — "A" the Donetsk coal basin, *3, 4, 7, 11* — "D" the Kuznetsk basin,
6, 8, 10, 12 — brown coal of Berezovsk Deposit, "B-2".

Comparison of dependencies of t_i (T_{am}) of "A" and "D" coals shows that in the range of moderate temperatures ($T = 900$–1150 K), the induction period of the anthracite coal-water particles is significantly higher than in the same particles of coals of mark "D" of the Kuznetsk coal basin. However, in the range of high temperatures ($T = 1150$–1500 K), the ratio of t_i is different. On the basis of the obtained results it is possible to conventionally distinguish two modes of combustion: high temperature and low temperature. Perhaps this is due to the fact that in the range of ambient temperature $T_{am} = 900$–1150 K, a major role in the ignition is played by a proportion of volatiles, which in the "D" coal is higher than in the "A" coal. At high temperatures ($T_{am} = 1150$–1500 K), the important are the effective thermal conductivity and the heat capacity of the CWF. The latter, for example, is lower in anthracite (1.3 times) compared with the coal of grade "D" [27, 28].

The data obtained from the numerical analysis in the form of dependences of ignition delay time on ambient temperature correspond to the conditions of furnaces of typical boiler units, i.e., high ambient temperature. For this reason, the experiments enabling the analysis of the regularities of these processes are difficult. The literature presents the results of experimental studies of CWF particles ignition but only under conditions of laser heating [29, 30]. To indirectly substantiate the reliability of the drawn theoretical conclusions we compared the results of solutions to problems (1)–(15), where the boundary condition (12) was changed to meet the conditions of the experiments [29, 30], with experimental data [29, 30]. Convective and radiant summand in the right-hand side was replaced by the laser radiation flux density q. Then, the condition (12) took the following form:

$$-\lambda_2 \frac{\partial T_2(r_0, t)}{\partial r} = q.$$

Due to the absence in [29, 30] of a complete description of all source data necessary for mathematical modeling, we performed the parametric analysis, whose results are shown in Fig. 2. As varied parameter there was the value q, which depends on the laser power, the cross-sectional area of the laser beam, and the distance to the particle. Figure 2 shows the results of numerical simulation and a straight line passing through the point corresponding to the experimental value t_i [29, 30]. Dependences shown in Fig. 2 give grounds to the conclusion that if in the experiments [29, 30], the value q has the range $5.5 \cdot 10^4 < q < 7.5 \cdot 10^4$ W/m²,
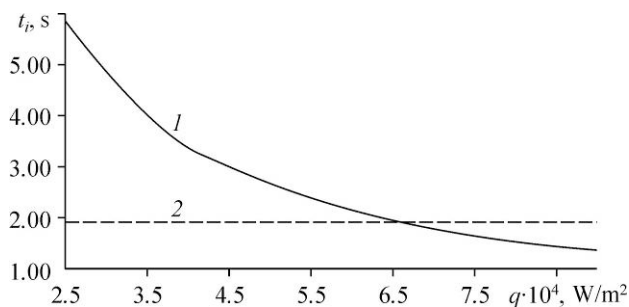
Fig. 2. Comparison of ignition delay time of the CWF particles ("D" from Kuznetsk basin)
obtained by numerical and experimental [29, 30] studies.

1 — numerical solution, *2* — straight line $t_i(q)$ passing through the point
corresponding to experimental value t_i [29, 30].

the discrepancy of the experimental and theoretical values of t_i is not beyond the confidence
intervals of the experiments on the ignition of the condensed substances. For comparison, it is
possible to provide random errors of measurement of ignition delay time for the group of high-
energy condensed substances determined in [31] at local heating by a single particle heated up
to high temperature. The relative standard deviations for t_i in [31] are ±20÷25 %. It may be
assumed with sufficient reliability that under the considered conditions of laser heating of CWF
particles, the error of t_i determination should be within the range close to the one established
in [31].

Figure 3 shows time dependences of the temperature of CWF particle surfaces with dia-
meter $d = 0.4 \cdot 10^{-3}$ m of three studied grades of coal. On each curve, three characteristic time
intervals can be distinguished. The first (before t_v) corresponds to a process of particles
dehumidification. It is worth noting the characteristic change of slope of the curve $T_s(t)$ at
the point (t_v, T_v). The latter corresponds to the time of complete removal of moisture from
the fuel. The change in the slope of the dependencies $T_s(t)$ is mainly determined by heat
conductivity of water saturated part of CWF. The second interval (before t_i) corresponds to
the heating and thermal decomposition of the dry coal. In this state, the thermal conductivity of
the latter is substantially less (compared with the first part) and, accordingly, the surface
temperature increases faster. At $t = t_i$, the condition of CWF ignition is performed, and
the surface temperature corresponds to the value T_i (ignition temperature of the particle).
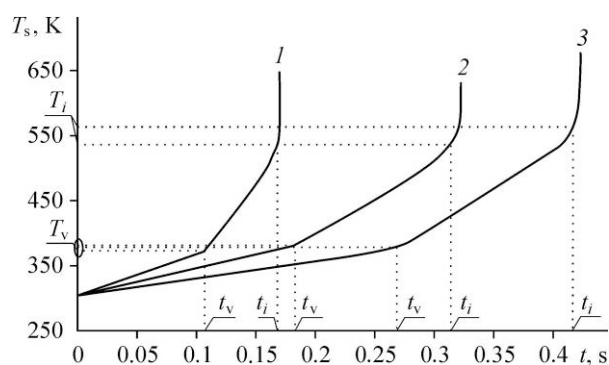

Fig. 3. Dependence of surface temperature (T_s) of the CWF particle with a diameter $d = 0.4 \cdot 10^{-3}$ m
on time t at ambient temperature $T_{am} = 1200$ K.

1 — brown coal of the Berezovsk basin of B-2 grade, *2* — coal A of the Donetsk coal basin,
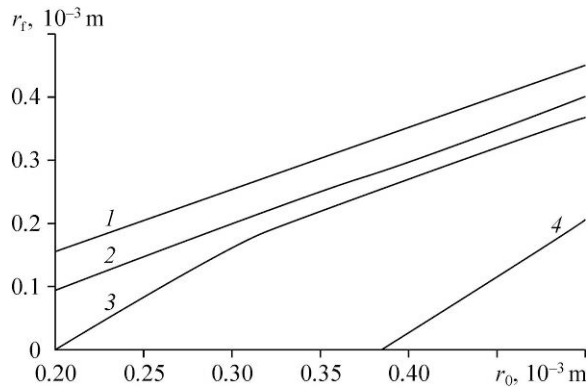*3* — coal of "D" grade of Kuznetsk basin.

r_f, 10^{-3} m

Fig. 4. Position of evaporation front in the moment of CWF particle ignition
(brown coal of Berezovsk deposit, grade B-2) depending on its dimensions
at different temperatures of ambient medium.
$T_{am} = 1500$ (*1*), 1200 (*2*), 1100 (*3*), 900 (*4*) K.

Further T_s increases to values corresponding to the CWF combustion. The third interval ($t > t_i$) corresponds to the process of stable combustion of coal-water particles.

The evaporation front position at the time of ignition is shown in Fig. 4. It may be noted that ignition of coal-water particles based on brown coal is possible prior to their complete "drying". Most likely, this is due to the low conductivity of such coal combined with a high content of volatiles.

Figure 5 shows the temperature distribution along the radius of the CWF particle at the time of ignition characterizing the state of fuel. It may be noted that in terms of "low temperature" mode ($T_{am} \leq 1100$ K), the ignition takes place only after complete dehumidification. At higher ambient temperatures ($T_{am} > 1100$ K), CWF ignites under conditions of continued evaporation. In the area of high temperature gradients, the formation of a layer with large thermal stresses becomes possible, and subsequent mechanical destruction of particles is similar to the mechanism of destruction of heat and fire protection materials [32].

In Fig. 5 it is easy to see the characteristic break on the curves 2 and 3, which corresponds to the boundary of the evaporation front. Due to an abrupt change of the thermal characteristics and heat absorption resulting from the phase transition, the slope of the curves changes. The temperature increases much faster.
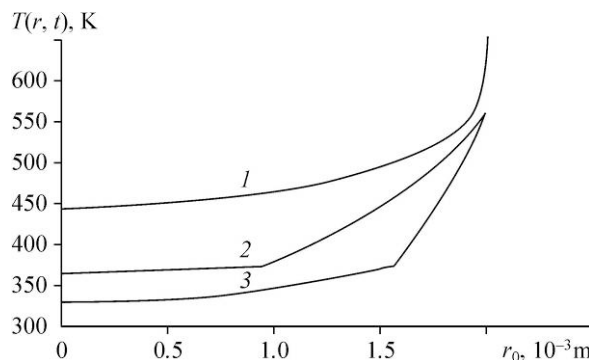
$T(r, t)$, K

Fig. 5. Temperature distribution over the CWF particle radius
(brown coal of Berezovsk deposit, grade B-2) in the moment of ignition.
$T_{am} = 900$ (*1*), 1200 (*2*), 1500 (*3*) K.

Conclusions

Numerical simulation of the main concurrent thermal (evaporation of water, thermal conductivity, and filtration) and thermochemical (pyrolysis of the organic part of fuel, chemical interaction of coke carbon and steam, oxidation of reaction products of the latter and thermal decomposition by oxygen) reactions has revealed a significant effect of thermophysical and thermochemical characteristics of the coals being the basic CWF.

It has been established that the CWF particles made from coals of mark "B" from the Berezovsk Deposit are ignited with less ignition time delay than the particles of the CWF from anthracite. Most likely, this is due to high (compared to anthracite) volatile content in brown coals. One more important factor is the role of higher thermal resistance of the mentioned CWF particles.

The numerical analysis has shown that the ignition modes of coal-water fuel particles from Berezovsk brown coal are possible in terms of their incomplete "dehydration". The process of such particles burning (in the context of the continued evaporation) is substantially different from the burning of dry coal.

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