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Influence of the Temperature Dependence of the Thermophysical Properties of Coal–Water Fuel on the Conditions and Characteristics of Ignition

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Abstract—The results of an experimental study and mathematical simulation of the ignition of coal–water fuel (CWF) particles, the main thermophysical characteristics of which (thermal conductivity (λ), heat capacity (*C*), and density (ρ)) depend on temperature, are reported. Based on the results of the numerical study, the influence of changes in the thermophysical properties upon the heating of the main bed of fuel on the conditions and characteristics of its ignition was analyzed. The ignition delay times (t_i) of CWF particles were determined under the typical furnace conditions of boiler aggregates. As a result of the mathematical simulation of the process of CWF ignition, it was established that the temperature dependence of thermophysical characteristics can exert a considerable effect on the characteristics and conditions of ignition. In this case, it was found that the ignition of coal–water drops is possible under the conditions of their incomplete dehydration. A good agreement of the theoretical ignition delay times of the CWF particles and the experimental values of t_i was established.

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INTRODUCTION

Basic obstacles to the fundamental development of the theory and practice of the use of solid fuels (primarily, coal) in power engineering are mainly related to the world economy, which is continuously changing in the recent decades [1–3]; in this case, changes in the prices of particular types of energy carriers are not an objective economic process. It is most likely that this is the reflection of the first forerunners of the future economic battles for territories with large deposits of the main liquid and gaseous energy carriers, which are of great interest for transnational corporations [6, 7].

The development of composite fuels based on coals, for example, coal–water fuels (CWFs), can become a basis for the replacement of oil and gas not only in small- and large-scale power engineering [8, 9] but also, possibly, (in medium-term planning) in truck and rail transport [10, 11]. However, an appropriate scientific and technical base for the fulfillment of the necessary research and development works is currently not available for the solution of the problem of the application CWFs. The results of experiments performed in the Former Soviet Union [12, 13] do not allow one to completely interpret the characteristics and conditions of the ignition of CWF particles. Note that the aim of the cited works [12, 13] was to study the process of CWF combustion. In this case, ignition processes did not receive sufficient attention. In this context, a main problem is to develop the theory of CWF combustion (including, first, steady ignition) as the basic stage of furnace or intrachamber (in internal combustion engines) processes based on CWFs.

Several approaches to the formulation of the problem of CWF ignition are well known [14, 15]; they are different in the dimensionality of factor spaces used in the development of physical and mathematical models for this complicated process. The formulations [16, 17] based on a set of nonstationary partial differential equations provide the greatest opportunities for the analysis of the conditions and characteristics of CWF ignition. The theoretical consequences obtained within the framework of models [18–20] create prerequisites for a conclusion on the possibility of the sta-

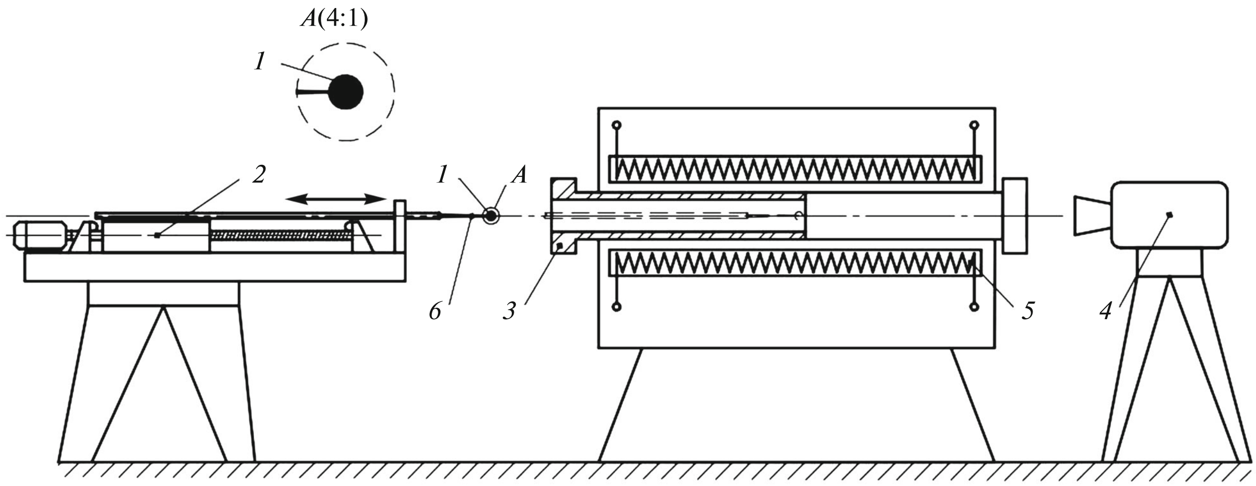

Fig. 1. Schematic diagram of the experimental setup: (*1*) CWF drop, (*2*) rectilinear manipulator, (*3*) hollow ceramic cylinder, (*4*) high-speed video camera, (*5*) electric heater, and (*6*) ceramic rod.

bilization of an ignition process and the subsequent combustion of CWF drops over a wide temperature range.

The studies [14–20] showed the influence of a group of significant factors (CWF properties [16], radiation heat exchange [17], and the shape of particles [18]) on the conditions and characteristics of the ignition of this substantially heterogeneous composition fuel. At the same time, it was established [19, 20] that high temperature gradients are formed in a CWF drop (or particle) during an induction period. They can exert a considerable effect on the properties of coals (primarily, on the thermophysical properties) [21]. For example, for this reason, a change in the thermal conductivity of the carbon skeleton of CWF can lead to significant changes in the duration of the induction period as a result of the more intense heat removal from the near-surface layer of the fuel into the depth (with an increase in the thermal conductivity with temperature). The influence of this factor was not analyzed, although it can play an important role under certain conditions.

The aim of this work was to analyze the influence of the temperature dependence of the thermophysical characteristics of CWF on the conditions and characteristic of the ignition of CWF particles.

EXPERIMENTAL

The ignition delay times of CWF particles were determined on an experimental setup (Fig. 1). CWF drops *1* were introduced by remotely controlled device *2* into hollow ceramic cylinder *3* heated to high temperatures (from 700 to 1200 K). The characteristic sizes of the test fuel particles were varied over a typical range (from 1.0×10^{-3} to 3.0×10^{-3} m). The processes of the thermal preparation and ignition of CWF particles were recorded with Phantom Miro M310 high-speed video camera *4* (video recording rate, 10000 fps).

The CWF drops prepared from the D coal from the Kuznetsk Basin were studied. Initially, the coal was ground in a ball-tube mill (to a fraction with a particle size of 40–80 μm), and the resulting dust was mixed with water; a cellulose-based additive (to 1 wt %) was added to the suspension for stabilization (to prevent the sedimentation of coal as a solid precipitate). For the determination of the characteristics and conditions of ignition, a series of six experiments was carried out at different values of T_e with the processing of the results of measurements by a least squares method [22]. The systematic error in the determination of the main measured parameters (T_e, t_i) was no greater than 5%. The confidence interval of the determination of t_i at a confidence coefficient of 0.95 did not exceed 14%.

Figure 2 shows the experimental dependence of t_i for CWF particles on ambient temperature. The diameter of the particles was varied in a range from 1.0×10^{-3} to 3.0×10^{-3} m. The experiments showed that T_e exerted a considerable effect on the characteristics and conditions of ignition: an increase in the ambient temperature from 600 to 1000 K led to a fivefold decrease in t_i. An analysis of curves *1–3* (Fig. 2) indicated their nonlinear shape, which can be explained by the essential influence of a set of the physicochemical processes of thermal preparation (thermal conductivity, moisture evaporation, thermal decomposition, and ignition) on the conditions and characteristics of the ignition of fuel. It is reasonable to believe that the evaporation of water is the most significant process of the thermal preparation of a CWF particle for ignition because of a great endothermic effect (to 2.5×10^6 J/kg).

Formulation of the Problem

In the system of differential equations that describe the main heat and mass transfer processes in a CWF particle, the solution region was divided (analogously to Syrodoi et al. [18]) into the two zones of the initial (moisture-saturated) fuel and the dry coal, through the porous structure of which water vapor and the thermal decomposition products of the organic matter of fuel were filtered into the region of ignition.

It was considered that, as a result of physicochemical transformations in the zone of high temperatures (above 80°C), the structure transformation of CWFs occurred to cause changes in both the fractions of main components (water, the coal framework, and the solid and gaseous products of the thermal decomposition of coal) and the thermophysical characteristics of the CWFs (λ, C, and ρ).

Different approaches to the description of the component composition of thermally decomposed or water-containing materials under the conditions of intense heating can be used (for example, according to Strakhov et al. [23]). However, the detailed specification (analogously to Strakhov et al. [23]) of the composition of the carbon residue (which included both carbon and incombustible mineral components) formed after the evaporation of moisture and the pyrolysis of organic matter is possible only with the use of a large body of initial data on the thermophysical characteristics of individual components. The determination of thermal conductivity, heat capacity, and density is the fairly complicated problem of an experimental study; therefore, in the formulation of the problem, we used a reaction scheme based on the hypothesis of the possibility of describing the thermophysical characteristics of CWFs with the use of additive expressions like those proposed by Strakhov et al. [23] for the thermal conductivity, heat capacity, and density of heterogeneous multicomponent systems.

The main difference of the formulation of the problem of ignition whose solution will be given below from published models [16–18] consists in the description of the temperature dependences of the thermal conductivity, heat capacity, and density of coal over the entire actually possible range of changes in the induction period. In addition to the main equations and boundary conditions [16–18], the mathematical model of the test process included the approximating expressions [21, 23]

$$\lambda_{\text{coal}} = (c_1 + dT)^{-1}, \quad (1)$$
$$(c_1 = 8.1763),$$

$$C_p(T) = A + BT + CT^2 + DT^3 + ET^4, \quad (2)$$

and the equation

$$\frac{d\rho}{d\tau} = (\rho - \rho_r)\, k \exp\left(-\frac{E}{RT}\right), \quad (3)$$

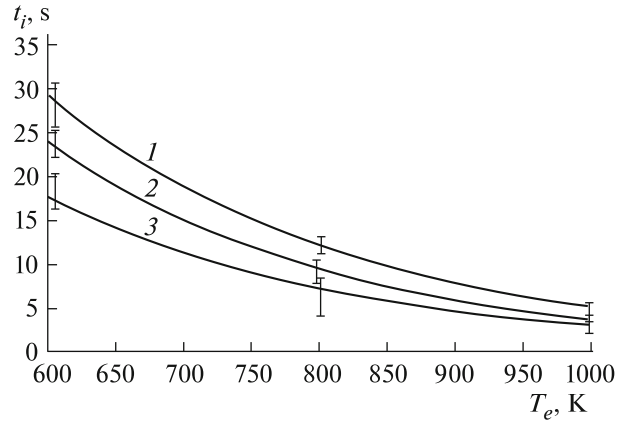

Fig. 2. Delay times of the ignition of coal–water fuel particles: δ = (*1*) 3 × 10^{-3}, (*2*) 2.5 × 10^{-3}, and (*3*) 3 × 10^{-3} m.

where $A = 0.89$ kJ kg^{-1} K^{-1}; $B = 5.5947 \times 10^{-3}$ kJ kg^{-1} K^{-2}; $C = -1.1742 \times 10^{-5}$ kJ kg^{-1} K^{-3}; $D = 1.6552 \times 10^{-5}$ kJ kg^{-1} K^{-4}; $E = 4.8502 \times 10^{-12}$ kJ kg^{-1} K^{-5}; R^4 = 0.9999; ρ_r is the coal density after the completion of the thermal decomposition process; and k and E are the preexponential factor and the activation energy, respectively, of the pyrolysis reaction of the organic matter of coal.

It is necessary to note that approximations like Eqs. (1)–(3), which were obtained as a result of experimental studies [21, 23], are a mathematical base for the estimations of the actual values of $\lambda = f(T)$, $C = f(T)$, and $\rho = f(T)$ with a certain error depending on the conditions of the experiments. However, as a rule, these estimations are sufficiently reliable, and they take into account the influence of the main significant factors on the thermophysical properties of coals.

The problem of heat and mass transfer in a spherical CWF particle in a period preceding the ignition is formulated in the form of a system of partial differential equations with appropriate boundary and initial conditions [16–18] and supplemented by expressions (1)–(3).

The formulated boundary-value problem was solved by a finite-difference method [24] with the use of an iterative algorithm analogous to that developed for the solution of the problems of ignition under the conditions of intense phase transformations [25] and a local thermal effect on a condensed substance [26]. For the verification of the results of a numerical simulation, we checked the conservatism of the difference scheme analogously to Kuznetsov and Sheremet [27]. The studies were carried out with the initial data given in the table.

We considered the ignition of a CWF particle based on D coal [28]. The thermophysical properties of the moist and dehydrated parts of the fuel were calculated

Thermophysical properties of coal [28]

Temperature (T), K	Thermal conductivity coefficient (λ), W m^{-1} K^{-1}	Heat capacity (C), J kg^{-1} K^{-1}
299	0.118	1052
373	0.141	1052
423	0.148	1351
473	0.160	1681
573	0.175	2099

taking into account the dependence on temperature (T) and the volume fractions of the components:

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

$$C_1 = \varphi_3 C_3 + \varphi_4 C_4(T), \quad C_2 = \varphi_3\lambda_4(T) + \varphi_5 C_5,$$

$$\rho_1 = \varphi_3\rho_3 + \varphi_4\rho_4(T), \quad \rho_2 = \varphi_3\rho_4(T) + \varphi_5\rho_5,$$

where the subscripts *1–5* refer to the initial (moisture-saturated) CWF, the dry fuel, water, coal, and vapor, respectively, and φ are the volume fractions of the components.

RESULTS AND DISCUSSION

Figure 3 shows the results of the comparison of ignition delay times obtained in a numerical simulation and experimentally. An analysis of $t_i(\delta)$ functions showed that the theoretical values of t_i were consistent with the experimental data in a range of particle sizes from 1.0×10^{-3} to 3.0×10^{-3} m. Note that, at relatively low temperatures (to 900 K), the difference between the experimental delay times of ignition and those calculated numerically increased. This was most likely due to the possible heat removal from the CWF particle through a ceramic rod on which it was attached (this effect was reported by Fuks [29]). In general, we can conclude that the published model [16–18] adequately describes the heat and mass transfer processes in the drop of CWF in a period that precedes the ignition of a coal–water slurry.

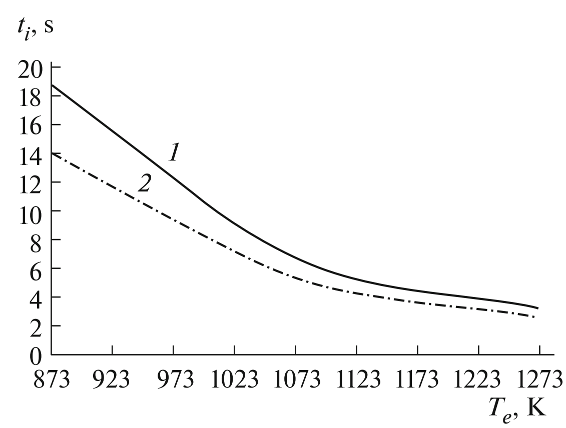

Fig. 3. Delay times of the ignition of coal–water fuel particles: (*1*) experimental data and (*2*) numerical solution.

Figure 4 illustrates the results of the solution of the problem of ignition for the sufficiently typical conditions of a thermal effect on the fuel particle: the ambient temperature was varied in the range T_e = 800–1300 K; the convective heat emission coefficient α was taken equal to 50 W m^{-2} K^{-1}; and the reduced emissivity was $\varepsilon = 0.7$.

An analysis of the experimental results showed that the ignition of CWF particles with a characteristic size of hundreds of microns is possible only at ambient temperatures higher than 700 K (in a real range of changes in the induction period time). In many respects, this was caused by the influence of the endothermic processes of water evaporation and vapor filtration to the heated fuel surface.

It can be clearly seen (Fig. 4) that each characteristic size of CWF particles corresponds to the limiting conditions of ignition in terms of the temperature of the environment. Differences in the delay times of ignition increase with decreasing T_e. At high T_e (≥1300 K), the values of t_i for the CWF particles with much different sizes (1 and 0.4 mm) were almost identical (within the limits of error in the initial data).

It is also possible to note significant differences in the times t_i of CWF particles with different diameters at identical relatively high ambient temperatures (Fig. 4). For example, at T_e = 800 K, an increase in the particle size by a factor of 2 led to an analogous increase in the values of t_i; this was caused by a consid-

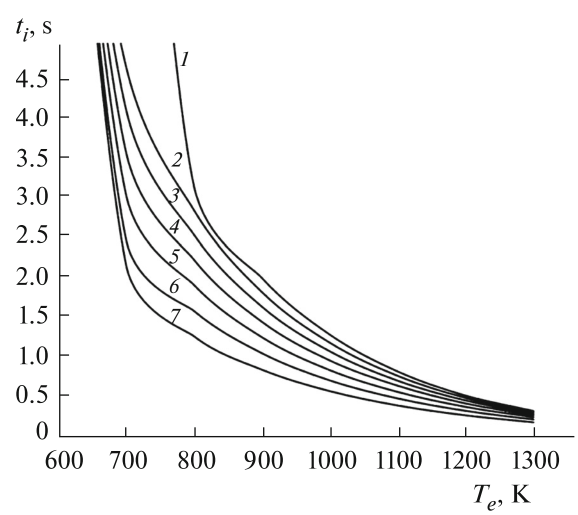

Fig. 4. Delay times of CWF ignition depending on ambient temperature for particles with diameters of (*1*) 1×10^{-3}, (*2*) 0.9×10^{-3}, (*3*) 0.8×10^{-3}, (*4*) 0.7×10^{-3}, (*5*) 0.6×10^{-3}, (*6*) 0.5×10^{-3}, and (*7*) 0.4×10^{-3} m.

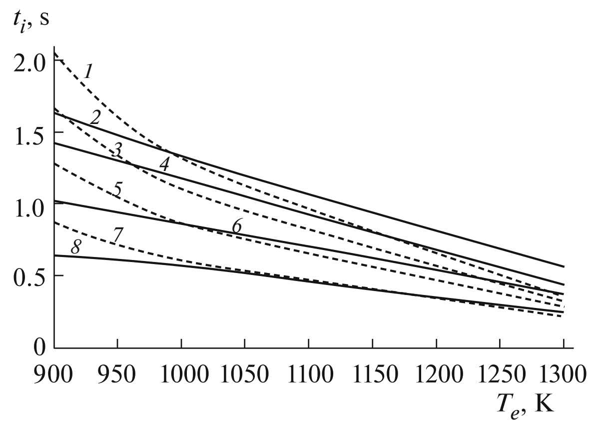

Fig. 5. Delay times of CWF ignition: (*1*, *2*) 1 × 10^{-3}, (*3*, *4*) 0.8 × 10^{-3}, (*5*, *6*) 0.6 × 10^{-3}, and (*7*, *8*) 0.4 × 10^{-3} m; dashed lines (*1*, *3*, *5*, *7*) with consideration for the temperature dependence of thermophysical properties and solid lines (*2*, *4*, *6*, *8*) without consideration for the temperature dependence of thermophysical properties.

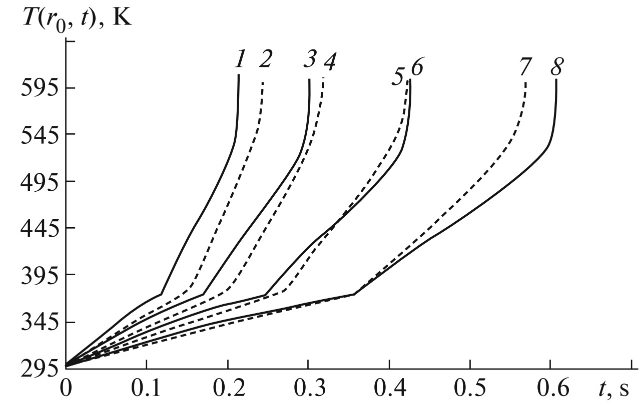

Fig. 6. The time dependence of the surface temperature of CWF particle with the diameter δ = 0.4 × 10^{-3} m: T_e = (*1*, *2*) 1300, (*3*, *4*) 1200, (*5*, *6*) 1100, and (*7*, *8*) 1000 K; (*1*, *3*, *6*, *8*) particles whose thermophysical properties depend on temperature; (*2*, *4*, *5*, *7*) particles whose thermophysical properties were taken constant.

erable increase in the consumption of energy for the heating and evaporation of water in the porous structure of the CWF particle.

Figure 5 shows the results of a comparison of the delay times of ignition with the temperature dependence of the thermophysical properties of coal–water fuel at the constant values of λ and C. It is evident that the values of t_i were insignificantly different for the particles of the same size in the range of ambient temperatures T_e = 950–1300 K; at lower T_e, the difference of t_i increased. Correspondingly, it is possible to distinguish between two regimes of ignition with a conditional boundary at T_e = 950 K: low-temperature and high-temperature ones. This is caused by the fact that, at higher ambient temperatures, the heating of particles occurs more intensely. Consequently, the temperature dependence of thermophysical properties manifests itself less clearly. Note that differences in the delay times of ignition were insignificant for small CWF particles ($r_0 \leq 0.4 \times 10^{-3}$ m). In the general case, it is possible to draw the conclusion that, in the range of ambient temperatures that are most frequently encountered in actual practice (T_e = 950–1300 K), a difference between the delay times of ignition is to 30% at λ = const and λ = λ(T).

Figure 6 shows the time dependence of the particle surface temperatures (T_p); it is possible to conditionally recognize a point of inflection for each temperature curve $T_p(t)$, which corresponds to the completion of a water removal process and, therefore, to the onset of the formation of a porous carbonaceous framework. As a result of the low thermal conductivity of this framework, an increase in the surface temperature of the particle occurred much more rapidly. It is remarkable that, at high ambient temperatures (T_e > 1000 K), the porous framework is formed more rapidly in the particles whose thermal conductivity depends on temperature in contrast to the particles whose values of λ were taken constant. Obviously, this is related to changes in the thermal conductivity with the temperature of coal.

Figure 7 shows the penetration depths of an evaporation front in the range of particle sizes from 0.05 × 10^{-3} to 0.4 × 10^{-3} m at the moment of ignition. It is evident that the coal–water particles, whose thermophysical properties depend on temperature, are set on fire even before the complete evaporation of moisture from the fuel. As noted above, this was most likely due to a change in the thermal resistance as a result of an increase in the temperature. Note that the particles whose thermophysical properties were taken constant were ignited only on the condition of complete drying.

The results obtained illustrate the possibility of reaching a higher level in the forecast of the influence of many factors on the ignition characteristics of complex heterogeneous systems such as coal–water fuel with the recognition of the majority of significant physical and chemical processes that occur in the CWF particle under the conditions of intense heating. The detailed description of individual heat and mass transfer processes in the regions with characteristic sizes smaller than δ = 1.0 × 10^{-3} m even in the solution of problems related to the ignition of relatively simple compositions such as CWF can create objective prerequisites for the analysis of the influence of structural and composition changes on both the integral (the delay time of ignition) and differential (maximum heating temperatures and temperature gradients) characteristics of a fuel ignition process.

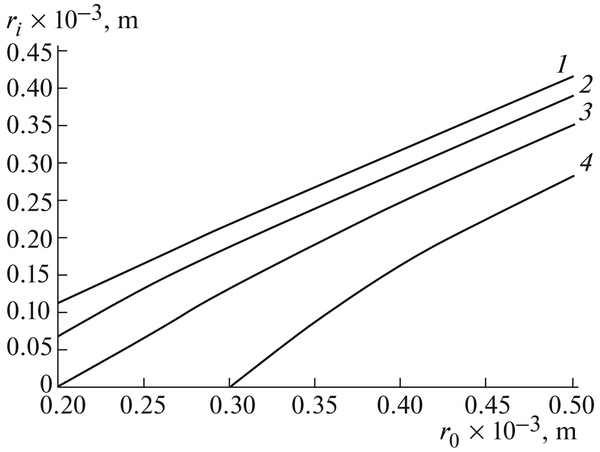

Fig. 7. Dependence of the coordinate of an evaporation front on particle size at the moment of ignition at ambient temperatures of (*1*) 1300, (*2*) 1200, (*3*) 1100, and (*4*) 1000 K.

CONCLUSIONS

We found that the temperature dependence of the thermophysical properties can exert a considerable effect on the characteristics and conditions of the ignition of CWF particles. This effect most significantly manifested itself at comparatively low ambient temperatures (lower than 1000 K). Under the high-temperature influence on the particle (T_e > 1000 K), the dependence $\lambda = \lambda(T)$ does not exert a considerable effect on the delay times of ignition. In this case, they can be calculated at λ = const.

The numerical analysis also showed that the duration of an induction period considerably increases at ambient temperatures lower than 800 K [30]. This was also confirmed by the experiments. In this case, the found delay times of ignition are beyond the scope of the optimum operation conditions of modern boiler aggregates.

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REFERENCES

1. Miljkovic, D., Dalbec, N., and Zhang, L., *Energy Economics*, 2016, vol. 55, p. 284.
2. Wilson, B. R., *Econometrica*, 2002, vol. 70, no. 4, p. 1299.
3. Tuzova, Y. and Qayum, F., *Energy Policy*, 2016, vol. 90, p. 140.
4. Weia, Y. and Guo, X., *Energy Economics*, 2016, vol. 56, p. 88.
5. Yue-Jun, Z. and Yao, T., *Economic Modelling*, 2016, vol. 55, p. 226.
6. Heinebck, B., *Oil and Security*, Stockholm: Stockholm Int. Peace Research Inst. Sveavgen, 1974, p. 166.
7. Rutledge, D., *Int. J. Coal Geology*, 2011, vol. 85, p. 23.
8. Khodakov, G.S., *Teploenergetika*, 2007, no. 1, p. 35.
9. Lan, G., Gong, X., Wang, Z., Zhao, L., Wang, Y., and Wang, M., *Energy*, 2016, vol. 96, p. 372.
10. Khodakov, G.S., Gorlov, E.G., and Golovin, G.S., *Khim. Tverd. Topl.* (Moscow), 2005, no. 6, p. 15.
11. Arun, K.W. and Murugan, S., J. Energy Inst., 2015, p. 1.
12. Delyagin, G.N., *Khim. Tverd. Topl.* (Moscow), 1973, no. 1, p. 127.
13. Ivanov, V.M. and Kantorovich, B.V., *Toplivnye emul'sii i suspenzii (Fuel Emulsions and Suspensions)*, Moscow: Metallurgizdat, 1963.
14. Huang, Z., *Proc. 8th Int. Symp. Coal Slurry Fuels Preparation and Utilization*, Orlando, 1986, part 1, p. 343.
15. Salomatov, V.V., Syrodoy, S.V., and Gutareva, N.Y., *IOP Conf. Series.: Mater. Sci. Eng.*, 66 012040.
16. Kuznetsov, G.V., Salomatov, V.V., and Syrodoy, S.V., *Combust., Explos., Shock Waves*, vol. 51, no. 4, p. 409.
17. Syrodoy, S.V., Kuznetsov, G.V., and Salomatov, V.V., *Thermal Eng.*, 2015, vol. 62, no. 10, p. 703.
18. Syrodoi, S.V., Kuznetsov, G.V., and Salomatov, V.V., *Solid Fuel Chem.*, 2015, vol. 49, no. 6, p. 365.
19. Syrodoy, S.V., Salomatov, V.V., and Gutareva, N.Y., *Eur. Ph. J. Web of Conf.*, 2015, vol. 82, p. 1.
20. Syrodoy, S.V., Gutareva, N.Y., and Salomatov, V.V., *Eur. Ph. J. Web of Conf.*, 2016, vol. 110, p. 1.
21. Wena, H., Lua, Jun-Hui, Xiaoa, Y., and Deng, J., *Thermochim. Acta,* 2015, vol. 619, p. 41.
22. Schenck, H., *Theories of Engineering Experimentations*, New York: McGraw-Hill, 1968.
23. Strakhov, V.L., Garashchenko, A.N., Kuznetsov, G.V., and Rudzinskii, V.P., *Combust., Explos., Shock Waves*, 2001, vol. 37, no. 2, p. 178.
24. Kuznetsov, G.V. and Sheremet, M.A., *Comp. Thermal Sci.*, 2011, vol. 3, no. 5, p. 427.
25. Glushkov, D.O., Syrodoy, S.V., Zhakharevich, A.V., and Strizhak, P.A., *Fuel Proc. Tech.*, 2016, no. 148, p. 224.
26. Kuznetsov, G.V., Mamontov, G.Y., and Taratushkin, G.V., *Khim. Fizika*, 2004, vol. 23, no. 5, p. 62.
27. Kuznetsov, G.V. and Sheremet, M.A., *Fluid Dynamics*, 2006, vol. 41, p. 881.
28. Agroskin, A.A., *Fizicheskie svoistva uglei (Physical Properties of Coals)*, Moscow: Metallurgizdat, 1961.
29. Fuks, N.A., *Isparenie i rost kapel'v gazoobraznoi srede (Drop Evaporation and Growth in a Gas Atmosphere)*, Moscow: Izd. Akad. Nauk SSSR, 1958.
30. Frank-Kamenetskii, D.A., *Diffuziya i teploperedacha v khimicheskoi kinetike (Diffusion and Heat Transfer in Chemical Kinetics)*, Moscow: Nauka, 1987.

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