

Modelling of heat and mass transfer to solve the problem of particle ignition water-coal fuel

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Abstract. The problem of particle ignition coal-water fuel (WCF) has been solved numerically, located at a high flow environment. Two different approaches to describe the physics of the process have been applied. According to the results of numerical simulation of the effect of the scale has been set about ambient temperature, the particle size on the inertia of the studied processes. A comparison of ignition delay times has been obtained using both methods of describing heat and mass transfer processes preceding fire.

1. Introduction

Use of coal-water fuel (WCF) in the heat is associated with the solution of a number of technical and technological problems [1]. One of the problems is the burning particles of WCF. The presence of water in such a structure leads to an increase in fuel required to initiate the combustion reaction heats the coal and hence significant increase of ignition delay time [2]. Known experimental data [1,2] on the ignition characteristics of particles WCF have been obtained only for sufficiently narrow ranges of parameters describing the process, and a small group of fuels.

A set of simplified formulations has been developed in the absence, until recently, the general mathematical models, methods and results of solving heat and mass transfer in the structure of WCF under intense heat [3-5]. Only one stage of a multistage process heat and mass transfer has been considered in a particle flowing coal-water fuel when heated in a stream of high-temperature gases in solving each of the problems [3-5]. The results of mathematical modeling of the processes preceding ignition WCF, based on simplified models [3-5] are the basis for assessing the true values of the ignition delay time of the particles of coal-water fuel (t_{ign}). It is advisable to compare these values with those obtained (t_{ign}) solving the problem of heat and mass in the formulation [11], taking into account the simultaneous occurrence at specific intervals throughout the group of basic physical and chemical processes [3-5] in the structure of WCF when heated to high temperatures. The joint implementation of "stages" [3-5] warming-up, evaporation, thermal decomposition of the organic portion of the coal and the subsequent ("secondary") products of chemical reactions physicochemical transformations between them in the appropriate temperature ranges are determined by a large temperature gradient across the thickness of the particle and continuous WCF state of the change in time as the removal of fuel from the heating surface.

Four problems have been solved in this paper. Three productions of which are given in [3-5] not resolved approximately analytically and numerically (finite difference method). Results of the solution in the form of dependency characteristic times of the processes of heating, evaporation and



thermal decomposition (preceding ignition) the ambient temperature are shown in Fig. 1-3. Figure 3 shows the main characteristics of the process — the ignition delay time t_3 (T_c).

2. Mathematical simulation

The mathematical model, the corresponding formulation of the problem [3-5] is described by the following system of differential equations:

- Energy equation for the initial (wet) of the fuel:

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

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

- Energy equation for “dehydrated” part WCF:

$$C_2 \rho_2 \frac{\partial T_2(r, t)}{\partial t} = \lambda_2 \cdot \left[\frac{\partial^2 T_2(r, t)}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial T_2(r, t)}{\partial r} \right] + Q_i \cdot \rho_2 \cdot \exp\left(-\frac{E}{R \cdot T(r, t)}\right). \quad (2)$$

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

The system (1.2) has been solved with the following boundary conditions and closing ratios:

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

$$-\lambda_1 \frac{\partial T_2(r_0, t)}{\partial r} = \alpha \cdot [T_c - T_2(r_0, t)] + \varepsilon \cdot \sigma \cdot [T_c^4 - T_2^4(r_0, t)]. \quad (3)$$

$$\frac{\partial T_1(0, t)}{\partial r} = 0. \quad (4)$$

The problem has been solved in a general setting heat and mass transfer in a particle of coal-water fuel in addition to problems [3-5]. The system of nonlinear no stationary differential equations with appropriate boundary conditions describing within the overall physical model the process under study is presented below:

- Energy equation for the initial (wet) of the fuel:

$$C_1 \rho_1 \frac{\partial T_1(r, t)}{\partial t} = \lambda_1 \cdot \left[\frac{\partial^2 T_1(r, t)}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial T_1(r, t)}{\partial r} \right]. \quad (5)$$

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

- Energy equation for “dehydrated” part WCF:

$$C_2 \rho_2 \frac{\partial T_2(r, t)}{\partial t} = \lambda_2 \cdot \left[\frac{\partial^2 T_2(r, t)}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial T_2(r, t)}{\partial r} \right] - \sum Q_i \cdot W_i - u_s C p_s \cdot \rho_s \frac{\partial T_2(r, T)}{\partial r}. \quad (6)$$

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

- The equation of chemical kinetics for the organic portion of the fuel:

$$\frac{\partial \eta_2(r, t)}{\partial t} = (1 - \eta_2(r, t)) \cdot k_0 \cdot \rho \cdot \exp\left(-\frac{E}{R \cdot T_1(r, t)}\right). \quad (7)$$

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

- Filtration equation for water vapor and gaseous products of thermal decomposition:

$$\frac{\partial p_s(r,t)}{\partial t} = \frac{m \cdot \xi \cdot Z}{K_p} \left(\frac{\partial p_s^2(r,t)}{\partial r^2} + \frac{2}{r} \frac{\partial p_s(r,t)}{\partial r} \right) \quad (8)$$

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

The boundary condition of the 4th kind has been used for the system (1-4) and (5-17) on the interface “original WCF — dry coal”:

$$\lambda_1 \frac{\partial T_1(r,t)}{\partial r} \Big|_{r=r_u-0} - \lambda_2 \frac{\partial T_2(r,t)}{\partial r} \Big|_{r=r_u+0} = Q_v \cdot W_v. \quad (9)$$

$$T_1(r_v;t) = T_2(r_v;t) = T_v$$

The system of equations (1-9) has been solved with the following boundary conditions and closing ratios:

$$0 < r < r_0; \quad T(r,0) = T_0; \quad P(r,0) = P_0; \quad \eta(r,0) = \eta_0;$$

$$-\lambda_2 \frac{\partial T_2(r_0,t)}{\partial r} = \alpha \cdot [T_c - T_2(r_0,t)] + \varepsilon \cdot \sigma \cdot [T_c^4 - T_2^4(r_0,t)] + \sum_i Q_i \cdot W_i. \quad (10)$$

$$\frac{\partial T_1(0,t)}{\partial r} = 0 \quad (11)$$

$$\frac{\partial P(r_v,t)}{\partial r} = \frac{K_p}{\nu} V_p(r_v;t) \quad (12)$$

$$p(r_0;t) = p_0 \quad (13)$$

Speed reversible reaction has been calculated from the following expression:

$$W_i = k_i \cdot c_i \cdot \rho_i \cdot \exp \left(-\frac{E}{R \cdot T(r,t)} \right) \quad (14)$$

Pyrolysis rate has been calculated using the following equation:

$$W_i = (1 - \eta(r,t)) \cdot k_i \cdot \rho_i \cdot \exp \left(-\frac{E}{R \cdot T(r,t)} \right) \quad (15)$$

ρ -density gaseous components has been determined from the equation of state:

$$\rho_i = \frac{P(r,t) \cdot \mu}{T(r_0;t) \cdot R} \quad (16)$$

Filtration rate has been determined by a pair of Darcy's law:

$$u = -\frac{K_p}{\nu} \frac{\partial P_p}{\partial r} \quad (17)$$

Notation, the initial temperature of T_0 — particles, K; T_c — ambient temperature, K; r_v —radius evaporation front, m; r_0 — outer radius of the particle, m; σ — constant blackbody radiation, $\frac{W}{m^2 \cdot K^4}$; α — convective heat transfer coefficient, $\frac{W}{m^2 \cdot K}$; λ_1 — thermal conductivity of the original WCF $\frac{W}{m \cdot K}$; λ_2 — dry thermal conductivity of the WCF, $\frac{W}{m \cdot K}$; C_1 —heat capacity of the initial part of WCF, $\frac{J}{kg \cdot K}$; C_2 —is the heat capacity of the initial part of the dry part of WCF, $\frac{J}{kg \cdot K}$; W_v — mass evaporation rate of water,

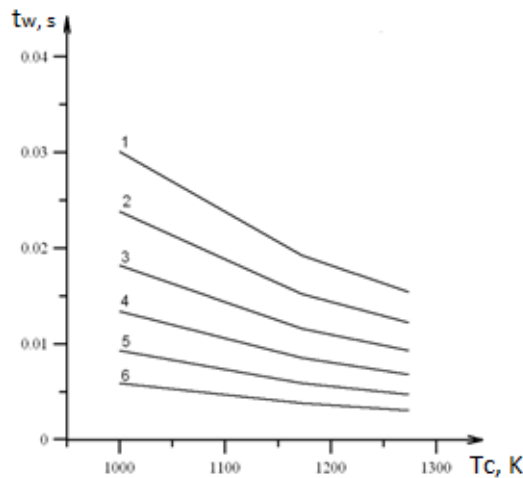


Figure.1. Dependence of the characteristic times for warm particle diameter WCF:

1- $0.9 \cdot 10^{-3}$ M; 2- $0.8 \cdot 10^{-3}$ M;
3- $0.7 \cdot 10^{-3}$ M; 4- $0.6 \cdot 10^{-3}$ M;
5- $0.5 \cdot 10^{-3}$ M; 6- $0.4 \cdot 10^{-3}$ M.

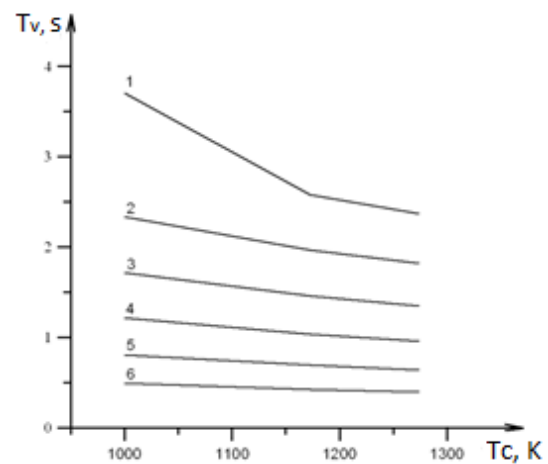


Figure.2. Dependence of the characteristic times for vaporization particle diameter WCF:

1- $0.9 \cdot 10^{-3}$ MM; 2- $0.8 \cdot 10^{-3}$ MM;
3- $0.7 \cdot 10^{-3}$ MM; 4- $0.6 \cdot 10^{-3}$ MM;
5- $0.5 \cdot 10^{-3}$ MM; 6- $0.4 \cdot 10^{-3}$ MM

$\frac{kg}{m^2 \cdot s}$; Q_V — thermal effect of the evaporation of water, $\frac{J}{kg}$; Q_i —thermal effect of the chemical reaction, $\frac{J}{kg}$; k_i —pre-exponential factor of the chemical reaction, $\frac{1}{s}$; E_i —activation energy of a chemical reaction, $\frac{J}{mol}$; u_s —filtration rate of water vapor, $\frac{m}{s}$; C_{p_s} —isobaric heat capacity of water vapor, $\frac{J}{kg \cdot K}$; ρ_s — vapor density, $\frac{kg}{m^3}$; p_s —vapor pressure in Pa; m —porosity; Z — degree of compressibility of water vapor; K_p — permeability porous structure, m^2 ; μ —molar mass of water, $\frac{kg}{mol}$; ν — kinematic viscosity of water vapor, $\frac{m^2}{s}$; C_i — concentration of the respective component of the chemical reaction; i — ordinal chemical reaction component.

Mass evaporation rate has been calculated from the expression:

$$W_V = W_0 \cdot \exp\left(\frac{Q_V \cdot \mu \cdot (T_1 - T_0)}{R \cdot T_0 \cdot T_1}\right)$$

Where: T_1 — evaporation temperature at the boundary, K; T_0 —fluid temperature corresponding to the point of freezing, K; W_0 — rate of evaporation at temperature, T_0 ; μ —molar mass of water vapor, $\frac{kg}{mol}$; R — universal gas constant, $\frac{J}{mol \cdot K}$.

The system (1) — (5) has been solved by finite difference method. The iterative algorithm has been used for solving nonlinear problems of heat and mass, designed for the simulation of intense evaporation of liquids [6, 7] and thermal decomposition of polymeric materials [8] under the intense heat. Choosing grid parameters should be adjusted to the specifics of the problem being solved (high temperature gradients and large rate of change of T) by analogy with [9, 10]. According to the results of solving the problem of heat conduction for a spherical particle WCF (Fig.1.) It can be noted that the characteristic time of warming up in the case of particles with a diameter of 0.4 mm to 0.9 mm, less than $3 \cdot 10^{-2}$ c.

Comparison of these values with the experimental data [3.4] allows us to conclude that the process of inert (non-thermal decomposition and evaporation of organic carbon) warming-up time is not more than 2.1% of the total duration. Consequently, the time period during stepwise consideration can be analyzed independently. Dripping processes (Fig.2.) extend substantially longer (about 100 fold) as

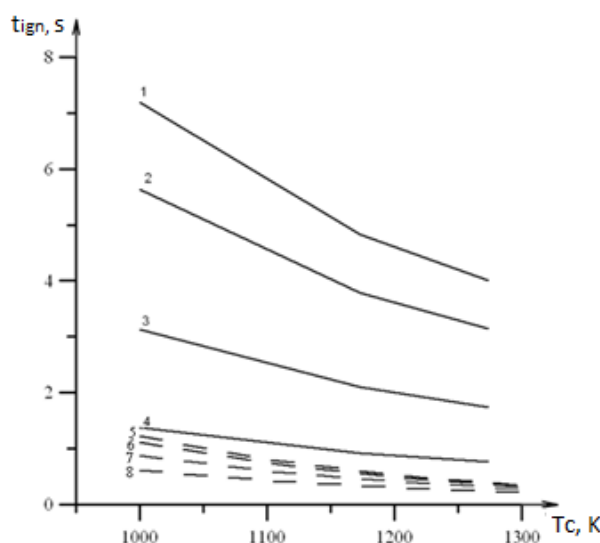


Figure.3. Dependence of the characteristic times of the ignition delay WCF particle diameter:
 1- $0.9 \cdot 10^{-3}$ mm; 2- $0.8 \cdot 10^{-3}$ mm; 3- $0.7 \cdot 10^{-3}$ mm; 4- $0.6 \cdot 10^{-3}$ mm; - solution of the system (1-4).
 5- $0.9 \cdot 10^{-3}$ mm; 6- $0.8 \cdot 10^{-3}$ mm; 7- $0.7 \cdot 10^{-3}$ mm; 8- $0.6 \cdot 10^{-3}$ mm; - solution of the system (5-17).

compared with the period of heating and the inert differ significantly from the total task time of ignition.

Figure 3 shows the results of numerical modeling of the test process as a dependency $t_{\text{ign}}(T_c)$ for particles of different diameters WCF obtained during the solution of (1-4) and (5-17). Comparison of the ignition delay time, resulting from the application of two different approaches to the description of heat and mass transfer in the particle coal-water fuel (Fig. 3) shows quite significant differences t_{ign} values. Last process, can be most likely due to the combined influence of these processes of heat transfer on the formation of the temperature field in the particle. For example, the evaporation of water takes place at any temperature up to the reflux temperature. The speed of evaporation and accordingly, the intensity of the absorption of energy in a small neighborhood of the evaporation surface are exponentially dependent on temperature. When relatively low temperatures, this heat sink is not taken into account in solving the problem of heat conduction only, the temperature at each point of the particles will be considerably higher WCF compared with the real one. As a result, the delay time t_{ign} is less than the true value. Similar effects will occur stepwise modeling in the future with increasing temperature and as you move the water and evaporation fronts beginning of thermal decomposition of the organic portion of the coal particles deep into the WCF. Furthermore, filtering products of vaporization through the porous structure is formed after the completion of the processes of evaporation and thermal decomposition would result in both a reduction of the absolute values of the temperatures at each point, and a decrease gradient T .

In conclusion, it should be noted that despite the fairly significant differences ignition delay times calculated using two different approaches to the above description of the basic processes occurring in coal-water fuel particle at high temperature, the simplified model [3-5] provide a generally acceptable for the initial stage analysis of numerical estimates of the values of t_{ign} .

References

- [1] Deljagin G.N. 1967. Problems in the theory of combustion of coal-water slurry in a stream of air. Conf. (Moscow).p. 45-55.
- [2] Deljagin G.N. 1969. In. Kinetics and Aerodynamics combustion processes. (Moscow).p.111-127.
- [3] Huang Z. et all. 1986. Proc. 8-th Int.. Symp. Coal Slurry Fuels Preparation and Utilization. (USA: Orlando.) V 1. p. 343-358.

- [4] Matthews K.J., Jones A.R. 1986. Proc. 8-th Int. Symp. Coal Slurry Fuels Preparation and Utilization. (USA: Orlando.) V **1**. p.. 388-407.
- [5] Salomatov V.V., Kravchenko I.V. 2007. Combustion and plasma chemistry. V. **5** no **3** p. 178-188.
- [6] Kuznetsov G.V., Stpizhak P.A. 2008. Journal of Engineering Thermophysics. V. **17**. no **3**. p. 244-252.
- [7] Kuznetsov G.V., Stpizhak P.A. 2009. Journal of Engineering Thermophysics. V. **18**. no **1**. p. 72-79 .
- [8] Strakhov V.L., Garashchenko A.N., Kuznetsov G.V., Rudzinskii V.P., 2001. Combustion, Explosion and Shock Waves. V. **37**, no **2**, p. 178-186.
- [9] Kuznetsov G.V., Mamontov G.Ya., Taratushkina G.V., 2004. Combustion, Explosion and Shock Waves. T **40**. no **1**. p. 70-76.
- [10] Kuznetsov, G.V., Mamontov G.Ya., Taratushkin, G.V. 2004. Chemical physics. V.**23**. no **5** p. 62-68.
- [11] Syrodoy S.V., Salomatov V.V., Kuznetsov G.V., 2013. Polzunovskii Vestnik. V. **4** no. **3** p. 28-33.