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Engineering Solutions for Clean Energy

NUMERICAL SIMULATION OF FIRE HAZARDOUS INTERACTION OF HOT PARTICLE WITH COAL DUST LAYER[*]

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Abstract

The mathematical model is designed to predict the characteristics of a fire-hazardous interaction of hot metal particles with a layer of coal dust. Such processes are difficult to control in practice, so the corresponding numerical simulation results are the basis for tightening fire management requirements. The developed mathematical model is represented by a system of nonlinear nonstationary partial differential equations with initial and boundary conditions. A numerical solution algorithm and the original program code have been developed in the MATLAB. The influence of parameters (initial temperature, shape, size) of a local heat source on the characteristics of gas-phase ignition of a layer of dispersed brown coal with a particle size of about 0.25 mm has been established.

Keywords: coal, hot particle, ignition, mathematical model, numerical simulation

1. Introduction

In recent years, the unstable situation in the world market of liquid and gaseous energy resources, as well as the increase in industrial production capacity are important factors in increasing the consumption of solid natural fuel (Arkhipov et al., 2014). Currently, fossil coals of various brands are widely used in industry not only as a solid fuel (Arkhipov and Putilov, 2009; Gagarin and Gyul'Maliev, 2009; Zekel et al., 2004), but also as raw

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materials for the production of synthetic liquid fuel (Krapchin and Potapenko, 2004; Maloletnev et al., 1992), gas (Potapenko, 2003; Shpirt et al., 2013), porous carbon (Kuznetsov et al., 2005) and building (Storozhenko et al., 2015) materials. In most technological combustion and recycling processes they use coals in powdered form with particles which have a size from several micrometers to several millimeters. Dispersed substances, containing volatile combustible components, present a high fire hazard at different stages of the preparation process, including grinding, reloading, transportation, drying, storage and others. Under such conditions, it is possible that dust deposits can ignite due to the effects of high-temperature gases (Fedorov and Khmel', 2005), static electric charges (Krainov and Baimler, 2002), heated bodies (El-Sayed and Khass, 2013). The study of interaction processes of such sources with crushed coals is of great importance for the prevention of fires in practice.

So far, a general theory of crushed coal layer ignition by a local heating source has not been developed. The purpose of this work is to develop this direction on the basis of study of the fact how the group of hot particles parameters influence on the ignition characteristics of the coal dust layer.

2. Mathematical model

Mathematical modeling is performed in the system "hot particle – crushed coal – air" (Fig. 1). The previously developed mathematical model was used for the research (Glushkov et al., 2018).

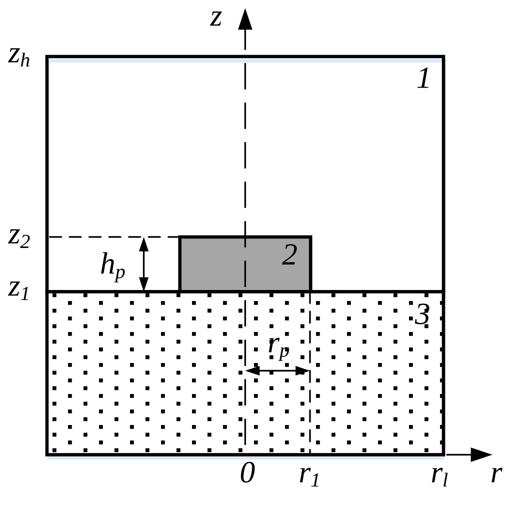


Fig. 1. The scheme of ignition problem solution area: *1* – air, *2* – hot particle, *3* – crushed coal

The following scheme of the investigated process is accepted. At the initial time, the hot particle, that is the ignition source with a temperature T_p, significantly higher than the ambient temperature T_0, is on the surface of the crushed coal layer. As a result of conductive heat transfer, the solid fuel near-surface layer is warmed up. With temperature increasing, the coal thermal decomposition rate increases, some volatile components are released. This process is most intensively progressing in the vicinity of the contact boundary with the hot particle, where the temperature reaches 500–600 K. From this region, the gaseous products of thermal decomposition are filtered in the direction of "crushed coal – air" boundary and are blown into the environment in small neighborhood of the local energy source base. In the conditions of fast inductive period, the thermal decomposition of coal leads to a decrease in the concentration of the organic part with a constant fuel volume. In gas environment, the combustible mixture is formed by mixing of volatile substances with air due to diffusion. Additional heating of the fuel mixed with the oxidizer occurs when this mixture moves along the side faces of the hot particle until the ignition conditions are reached.

The following ignition conditions (Glushkov et al., 2013; Glushkov et al., 2014) corresponding to the classical criteria of Y.B. Zeldovich, D.A. Frank-Kamenetskii, A.A. Kowalski and V.N. Vilanova are accepted, as well as taking into account the peculiarities of spatial-temporal heterogeneity of physical-chemical processes in the gas-phase model of combustion initiation:

1. The heat released by the oxidation reaction of volatile substances is greater than the energy withdrawn from the hot particle into the solid fuel and gas mixture.

2. The temperature of gas mixture in the zone of intensive oxidation reaction development exceeds the local energy source initial temperature.

The mathematical model of the investigated process (Glushkov et al., 2018) is a system of nonlinear unsteady differential equations of energy (for coal dust and gas mixture), thermal conductivity (for hot particles) and diffusion (for gas mixture) in partial derivatives with corresponding initial and boundary conditions. Mass rates of oxidation reactions of the gas mixture and thermal decomposition in the heated region of the crushed coal layer were calculated according to the Arrhenius law (Frank-Kamenetskii, 2015). The algorithm for numerical solution of the equations system combines finite difference methods, a locally one-dimensional method, an iteration method, and a run method.

Verification of the developed mathematical model and evaluation of the numerical study results reliability is carried out by checking the conservatism of the difference scheme used. The error of energy conservation law in the ignition problem solution area (Fig. 1) was calculated according to Eq. (1):

$$\delta_Q = \frac{Q_1^{ign} + Q_1^{ox} + Q_2^{ign} + Q_3^{ign} - Q_3^{dec}}{Q_2^0 + Q_1^{ox} - Q_3^{dec}}, \qquad (1)$$

where Q_1^{ign} is the heat accumulated by the gas mixture due to the heat capacity at $t=t_d$, J;

Q_1^{ox} – heat released from the volatile matter oxidation at $t=t_d$, J;

Q_2^0 – the heat of the energy source at $t=0$, J;

Q_2^{ign} – the heat of the energy source at $t=t_d$, J;

Q_3^{dec} – heat spent on coal thermal decomposition at $t=t_d$, J;

Q_3^{ign} – heat accumulated by solid fuel due to heat capacity at $t=t_d$, J.

Here t_d is the ignition delay time, i.e. the time from the beginning of the coal heating in contact with the hot particle to the gas-phase ignition of the combustible gas mixture in the vicinity of the particle. The ignition characteristics were calculated at steps in spatial coordinates $\Delta r=\Delta z=100$ µm and time $\Delta t=10$ µs. In the vicinity of the intense thermal coal decomposition zones and the gas mixture oxidation, the difference grid thickened, the step decreased to 5 microns. The energy balance error was $\delta_Q<2\%$ with variation of the heating source initial temperature in a sufficiently wide range T_p=800–1500 K.

Testing of the used numerical methods and elements of the developed algorithm for solving a system of nonlinear unsteady partial differential equations with corresponding initial and boundary conditions is also carried out on the example of conductive thermal conductivity problems with matter chemical reaction.

The hot particle parameters values, the problem solving area, thermal and physical characteristics of substances and materials, as well as the kinetic parameters of reactions of the coal thermal decomposition and volatile components oxidation are given in Table 1. It was assumed that coal thermal decomposition and volatile substances oxidation produce chemical reactions with effective kinetic characteristics (pre-exponential factor, activation energy, thermal effect). Numerical studies were performed for the typical 2B brown coal.

Small disk- and parallelepiped-formed metal particles heated to high temperatures were considered as local energy sources.

Table 1. Values of constants used in mathematical modeling

Parameter	***Designation***	***Value***
Solution area dimensions	r_l, z_h	10–20 mm
Hot particle sizes	r_p, z_p	5–10 mm
Initial temperature of coal and air	T_0	300 K
The source initial temperature	T_p	1100–1500 K
Air density	ρ_o	1.161 kg/m^3
The air heat capacity	C_o	1190 J/(kg·K)
The air thermal conductivity	λ_o	0.026 W/(m·K)
The steel density	ρ_2	7831 kg/m^3
The steel heat capacity	C_2	470 J/(kg·K)
The steel thermal conductivity	λ_2	49 W/(m·K)
The coal density	ρ_3	1200 kg/m^3
The coal heat capacity	C_3	1440 J/(kg·K)
The coal thermal conductivity	λ_3	0.149 W/(m·K)
The volatiles density	ρ_f	0.5 kg/m^3
The heat capacity of volatile substance	C_f	1132 J/(kg·K)
The thermal conductivity of volatile substance	λ_f	0.03 W/(m·K)
The thermal effect of coal thermal decomposition	Q_3	2.55·10^6 J/kg
The pre-exponential factor of coal thermal decomposition	k_3	10^7 1/s
The activation energy of coal thermal decomposition	E_3	195·10^3 J/mol
The thermal effect of volatile substances oxidation	Q_1	5.52·10^7 J/kg
The pre-exponential factor volatile substances oxidation	k_1	10^4 1/s
The activation energy of volatile substances oxidation	E_1	77·10^3 J/mol
Diffusion coefficient	D_0	0.56·10^{-4} m^2/s
The universal gas constant	R_t	8.314 J/(mol·K)

Below there are the results and the analysis of the most significant factors influence (initial temperature, size, the local heating source shape) on the conditions and on the crushed coal ignition characteristics. When varying the parameters of the hot particle, it was assumed that the heat content of the energy sources is given by Eq. (2):

$$Q_2^0=\rho_2 C_2 V_2(T_p-T_0), \tag{2}$$

where:

ρ_2 is the density of the material, kg/m^3; C_2 is the heat capacity of the material, J/(kg·K); V_2 is the particle volume, m^3; T_p is the initial temperature of the particle, K; T_0 is the ambient temperature, K.

3. Results and discussion

Previously (Zakharevich and Ogorodnikov, 2013a, 2013b; Zakharevich and Bogomolov, 2015), the ignition process stability of a dispersed coal layer in interaction with a single particle heated to high temperatures was experimentally established. The studies were performed in a rather narrow range (1313–1473 K) of the local source initial temperature variation in the disk form with dimensions r_p=3 mm, z_p=3–7 mm. Undoubtedly, the experimental data (Zakharevich and Ogorodnikov, 2013a, 2013b; Zakharevich and Bogomolov, 2015), are the basis to develop the theoretical positions connected with the dispersed solid fuels combustion initiation processes under the conditions of local heat by the sources of limited energy capacity, which subsequently can be used in practice, for example, to prevent accidents. Therefore, it seems appropriate to study theoretically conditions and characteristics of the dispersed solid fuel ignition with variation in a wide range of the main hot particle parameters (initial temperature, shape, size).

Table 2. Characteristics of 2B brown coal of Shiwei-Ovoo deposit in Mongolia (Zavorin et al., 2014)

Technical analysis				***Ultimate analysis***				
W^a, %	***A^d, %***	***V^{daf}, %***	***Q^r_s, MJ/kg***	***C^{daf}, %***	***H^{daf}, %***	***N^{daf}, %***	***S^{daf}, %***	***O^{daf}, %***
28	12.3	51.54	14.82	73.27	4.63	0.88	0.93	20.3

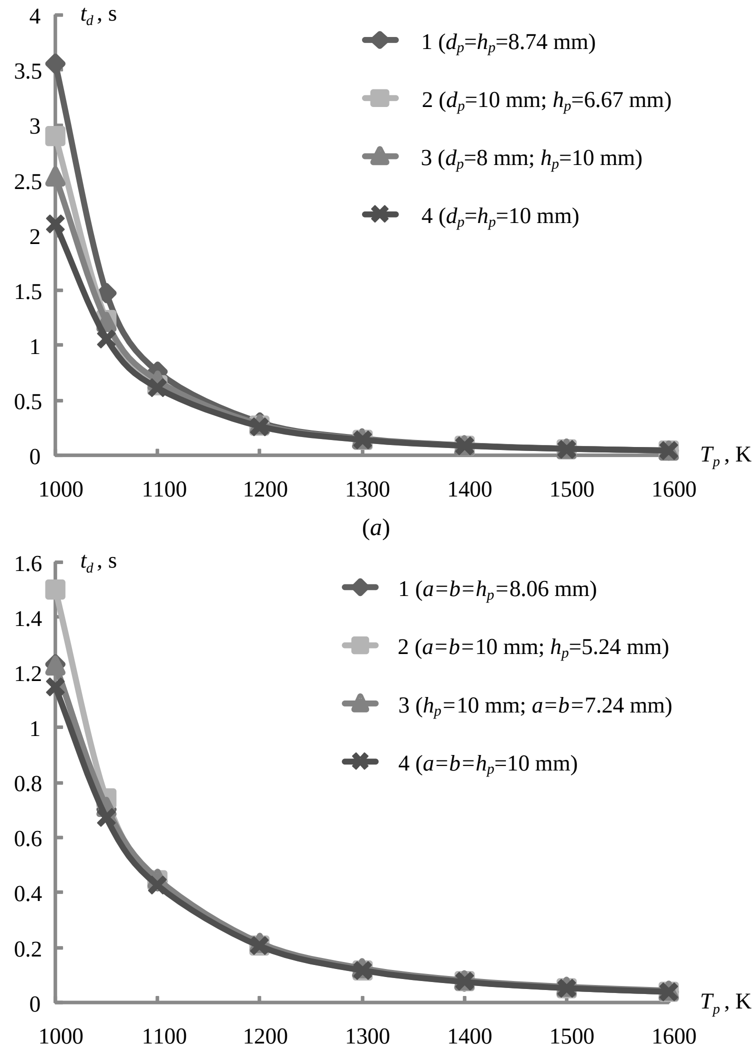
Table 3. Modeling results

	Disk sizes				***Parallelepiped sizes***			
T, K	***d_p=h_p=8.74 mm***	***d_p=10 mm h_p=6.67 mm***	***d_p=8 mm h_p=10 mm***	***d_p=h_p=10mm***	***a_p=b_p=h_p=8.06 mm***	***a_p=b_p=10 mm h_p=5.24 mm***	***a_p=b_p =7.24 mm h_p=10 mm***	***a_p=b_p=h_p=10 mm***
1000	3.5588	2.9035	2.5307	2.0984	1.2313	1.5008	1.2237	1.1475
1050	1.4761	1.2275	1.212	1.0595	0.7041	0.7406	0.7096	0.6711
1100	0.7631	0.6412	0.6799	0.6114	0.4431	0.4442	0.4485	0.4269
1200	0.3022	0.2659	0.2832	0.2645	0.2126	0.2081	0.2155	0.2067
1300	0.1563	0.1422	0.1494	0.1421	0.1217	0.1188	0.1232	0.1187
1400	0.0947	0.0881	0.0916	0.0881	0.0785	0.0768	0.0794	0.0768
1500	0.0641	0.0604	0.0623	0.0604	0.0553	0.0541	0.0558	0.0541
1600	0.0466	0.0444	0.0456	0.0444	0.0413	0.0403	0.0417	0.0405

Mathematical modeling (Glushkov and Zakharevich, 2013) of the crushed coal ignition by a heated disk-formed steel particle is performed in a cylindrical coordinate system (Fig. 1), by a parallelepiped-formed particle – in the Cartesian coordinate system. As a solid fuel, a typical 2B Shiwei-Ovoo Brown coal of Mongolia deposit was selected, which is similar in thermal properties to the widespread 2B and 3B energy coals of the Kansk-

Achinsk basin (Berezovsky and Irsha-Borodino deposits), of the Azeisky deposit of the Irkutsk basin in Russia, as well as of the Baganur deposit in Mongolia (Zavorin et al., 2014). Characteristics and component composition of 2B and 3B brown coal varies in rather narrow ranges (Zavorin et al., 2014): moisture content $25<W^a<40\%$; dry mass ash content $5.7<A^d<12.5\%$; volatile content $40.3<V^{daf}<53.7\%$; combustion heat of the lower working mass $14.6<Q^r_s<15.99$ MJ/kg; carbon content $71.2<C^{daf}<74.2\%$, hydrogen content $4.6<H^{daf}<5.5\%$, nitrogen content $0.88<N^{daf}<1.3\%$, sulfur content $0.26<S^{daf}<1.18\%$, oxygen content $19<O^{daf}<22.28\%$. Solid natural fuels key features (in the initial state) of Shiwei-Ovoo deposit are shown in Table 2 (Zavorin et al., 2014).

They set the dependencies (Fig. 2) in ignition delay time t_d of crushed coal from the initial temperature of a hot disk-formed particle with size varying d_p and h_p and of a cube-formed particle with size varying a_p, b_p and h_p.



(*b*)

Fig. 2. The dependence of ignition delay times of crushed coal from the initial temperature of particles with different sizes: (*a*) in the form of a disk; (*b*) in the form of a cube

These parameters of the local source determine its heat content according to Eq. (2). At the initial time, the heat content of hot particles in the disk form is correlated as 1 (d_p=8.74 mm, h_p=8.74 mm) : 1 (d_p=10 mm, h_p=6.67 mm) : 1 (d_p=8 mm, h_p=10 mm) : 1.5 (d_p=10 mm, h_p=10 mm); cube – shaped as 1 (a_p=b_p=8.06 mm, h_p=8.06 mm) : 1 (a_p=b_p=10 mm, h_p=5.24 mm) : 1 (a_p=b_p=7.24 mm, h_p=10 mm) : 1.9 (a_p=b_p=10 mm, h_p=10 mm). It is revealed that with increase in Q_2^0 (due to the size when T_p=const), the most significant decrease (to 41 %) of the ignition delay time is typical for the range of relatively low initial temperatures of the source (T_p=1100–1200 K), close to the limit (T_p=1030 K) conditions of solid fuel combustion initiation. At higher T_P values, this factor has less influence (up to 25%) on the reduction of the induction period duration. The obtained result allows us to conclude that at a relatively high heat content of hot particles (at T_p>1400 K), the change in the heating source size in the range d_p=8–10 mm, h_p=6–10 mm in a disk form and a_p=b_p=7–10 mm, h_p=5–10 mm in a cube form, under other equal conditions, has less significant effect on the intensity of fast-flowing (t_d<0.1 s) physical and chemical processes. At T_p<1300 K, the duration of inert crushed coal heating increases. Under such conditions, with identical initial temperature of sources with different heat content (curves *1* and *4* on Fig. 2), the ignition delay times increase for particles with a lower Q_2^0. In this case, as a result of heat removal to the environment (coal and gas), metal particles cool more intensively. At the time of ignition, their temperature is 20–40 K below than the temperature of particles with higher heat content (at identical T_p).

Also, according to the results of numerical analysis, it was found that for two hot particles with equal heat content Q_2^0 at identical initial temperatures of the source T_p, the ignition delay times may differ (curves *1*, *2* and *3* on Fig. 2) due to the different ratio of the areas of heating source surfaces bordering with the coal S_3 and the gas medium S_1. In the region of relatively high initial temperatures (T_p>1350 K) t_d are minimal at large values of S_3. In this case, the heat flow on the near-surface layer of the crushed coal exceeds the same value for smaller values of S_3, which leads to more intense heating, thermal decomposition of coal, release of volatile components and, accordingly, to a decrease in the ignition delay time. At the local source temperatures close to the limit conditions of combustion initiation (T_p<1250 K) t_d are minimum at large values of S_1 (due to the increase in h_p) in contrast to a high temperature area. This can be explained by the fact that with a relatively small heat content of hot particles, the induction period duration (t_d→1 s) increases. The heating depth of the crushed coal surface layer to the intense thermal decomposition temperature (T_3=500–600 K) is 0.4–0.6 mm. Under such conditions, the concentration of volatile substances in the vicinity of the local source is high. The ignition delay time corresponds to the duration of gas mixture heating when it moves along a side face of the particle until the ignition moment. At low h_p heating of the volatile substances mixture with an oxidizing agent, until all the conditions of combustion initiation are met, can be achieved only on the particle, thus increasing the ignition delay time as compared with the case of bigger h_p when the ignition is realized in the neighborhood of particle side face.

The revealed pattern of change in the ignition zone position is also established with the local source initial temperature varying. They found three ignition modes (Fig. 3), characterized by interrelated parameters of the local energy source (initial temperature) and the ignition process (delay time, the location of the oxidation reaction zone in the vicinity of the hot particle).

The first mode (Fig. 3a) is characterized by large temperature gradients on the border of the "hot particle – crushed coal". For a small time interval t≈0.1 s, a thin near-surface layer is heated to the temperature of intense thermal decomposition. The volatile substances, formed in the vicinity where the hot particle contacts with coal, are filtered in the direction of the coal heated surface of and are blown into the air in the vicinity of the local energy source base (Fig. 3a). Due to sufficiently high concentrations and temperatures of the thermal decomposition products of solid fuel in this zone, the ignition conditions of volatile substances gas mixture with air are achieved.

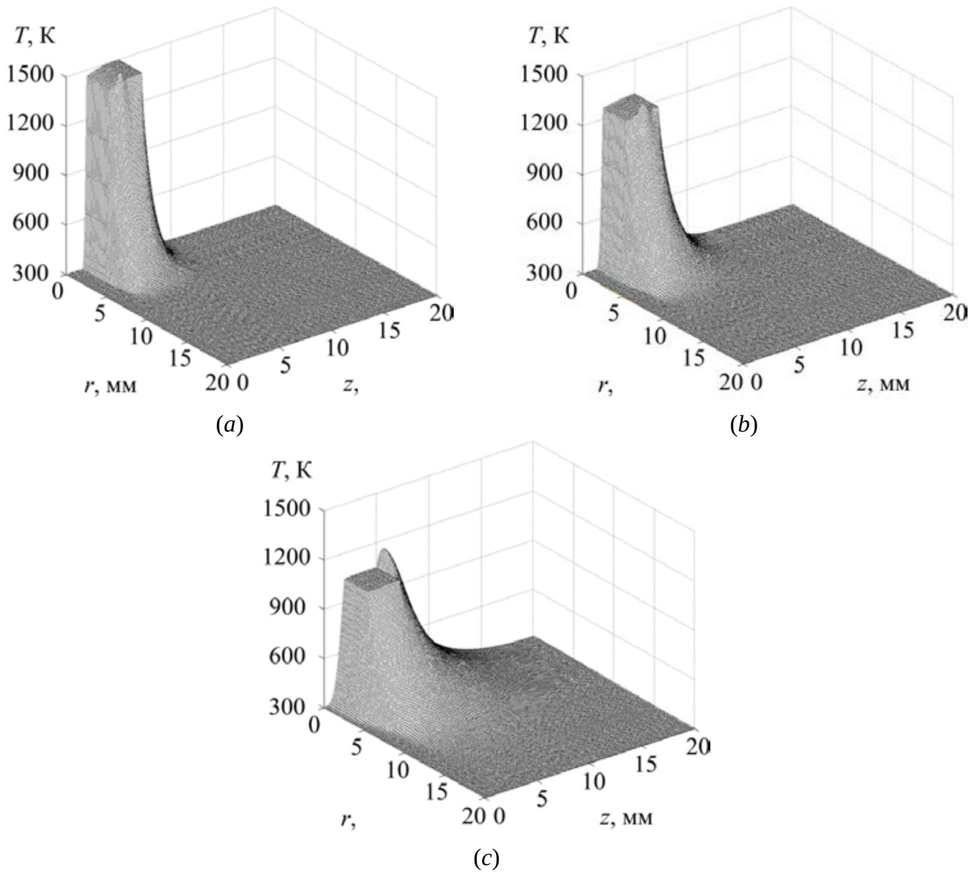


Fig. 3. Typical temperature fields (T, K) at the time of ignition of crushed coal with a disk-shaped particle (r_p=z_p=5 mm): (a) – t_d=0.041 s at T_p=1500 K; (b) – t_d=0.137 s at T_p=1300 K; (c) – t_d=1.281 s at T_p=1100 K

Fig. 3b shows the fields of temperature and concentrations in terms of the combustion initiation second mode. Compared to the first regime the lower temperature gradients on "hot particle – crushed coal" boundary are clearly visible. In this case, the heat transfer processes in the near-surface layer and heat and mass transfer in the gas medium have a significant impact on the ignition characteristics. With a decrease in the local energy source initial temperature, the influence of this factor increases, which leads to an increase in the delay time and to a shift in the ignition zone position in the gas mixture direction. Since ignition occurs at certain temperatures of the gas mixture and the concentration of volatile components in it, in conditions of moderate thermal coal decomposition, heating of the gas mixture to higher temperatures is required. This occurs when a mixture of volatile substances with oxygen moves along the side-faces of the hot particle ($r \rightarrow r_1$, $z_1 < z < z_2$, see Fig. 1).

In conditions of the third ignition mode (Fig. 3c) the local energy source temperatures are close to the values corresponding to the limiting conditions of the process. The relatively low temperature of the hot particle causes a long warm-up of the near-surface layer up to the moment when one meets the conditions of intense thermal decomposition and prolonged warm-up of the gas mixture up to volatile substances ignition. In this case, even with low thermal crushed coal conductivity, there is a significant removal of heat from the local energy source deep into the dust layer. It should be noted that during the time t_d>1 s the particle temperature decreases by more than 100 K, and the surface coal layer warms up to the temperature of intense thermal decomposition to a depth of about 0.5 mm. The motion of volatiles and air mixture along the hot particle side faces does not reach ignition conditions. Therefore, the gas mixture heating to a high temperature and the combustion initiation occur above the particle (Fig. 3c).

4. Concluding remarks

According to the numerical modeling results it was found that the ignition of the crushed brown coal, which is quite typical for heat power engineering, is possible when a small-sized particle (several millimeters) heated to the temperature about 1100 K drops on a layer of such fuel.

The analysis allows us to conclude that at relatively large sizes (more than 5 mm) and high initial temperatures (T_p>1400 K) of hot particles – ignition sources, the ignition conditions of the crushed coal layer are realized at small values of delay times (t_d<0.1 s), and the influence of the heating source configuration on the conditions and characteristics of the initiation process is insignificant.

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