Modeling of the flame propagation in coal-dust- methane air mixture in an enclosed sphere volume.

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Abstract. The results of the numerical simulation of the flame front propagation in coal-dust-methane-air mixture in an enclosed volume with the ignition source in the center of the volume are presented. The mathematical model is based on a dual-velocity two-phase model of the reacting gas-dispersion medium. The system of equations includes the mass-conversation equation, the impulse-conversation equation, the total energy-conversation equation of the gas and particles taking into account the thermal conductivity and chemical reactions in the gas and on the particle surface, mass-conversation equation of the mixture gas components considering the diffusion and the burn-out and the particle burn-out equation. The influence of the coal particle mass on the pressure in the volume after the mixture burn out and on the burn-out time has been investigated. It has been shown that the burning rate of the coal-dust methane air mixtures depends on the coal particle size.

1. Introduction

The experimental studies on the influence of the coal-dust on the ignition characteristics of gas mixtures have been conducted for several decades. In the studies the mixture proportions (the methane and coal particle mass content) and the reaction places (a spherical bomb, a tube, dust-laden flame) have been varied, the influence of the additives (deterrents and retarders) on the burning characteristics of the hybrid mixtures has been analyzed.

It has been shown in [1] that the reactive gas and coal dust mixture is able to explode under the low concentration of the coal dust in the air. The data in [1] show that the coal dust in the air and the methane air mixture in separate trials under the chosen concentrations in the air are not able to explode, but its mixture can be highly explosive. The flame propagation velocity in the methane air mixture increases with the presence of the small coal dust particles [2]. The experimental study on the burning of the coal dust and 6.5% methane-air mixture in a spherical volume has been carried out in [3]. The authors in [3] indicate the significant influence of the coal dust particles on the burning characteristics of the reactive gas mixtures. The rate of the pressure growth in the volume with the presence of the coal dust particles in the mixture is higher than that without the particles. In [4] for the coal dust-air mixture it has been shown theoretically that under the normal conditions the mixture burning become possible by adding a small amount of methane or by preheating the burner walls. The influence of the coal dust particles on the hybrid mixture burning rate has been investigated in [5]. The results have shown that for the laminar flames the small size particles decrease the normal velocity of the flame front.

In [6] the authors proposed the physical-mathematical model of the ignition and the detonation burning of the coal dust suspension in the air. The research on the comparison of the obtained results from one-velocity model and dual-velocity models has been carried out. It has been observed in [7] that at the low concentrations of the fuel in the mixture the presence of the reacting particles increase the velocity of flame front propagation.

The experimental and theoretical researches have shown that the burning characteristics of the hybrid mixtures significantly depend on the size of the reacting particles. The burning process is affected by the surrounding conditions. One of the methods determining the burning characteristics of the coal dust and reactive gas mixture is the burning in a spherical volume. In the present paper the numerical simulation of the flame front propagation in the coal-dust methane–air mixture in the enclosed spherical volume has been carried out. The aim of the study was to determine the mass and the particle size influence on the rate of the pressure growth.

2. Mathematical model

It is supposed that the monodisperse suspension of the coal dust particles which mass is m_{pyl}, and the particle radius is r_k and 1% methane-air mixture are located in the enclosed spherical volume V with the radius r_S. The ignition of the mixture is executed by the hot spot in the center of the volume with the radius r_0. The heat transfer to the surrounding environment is neglected. The diffusion and the heat transfer coefficients depend on the temperature [8]. The gas motion caused by the heat expansion due to the rising temperature is taken into account. There are two parallel reactions in the mixture, the first is the exothermic chemical reaction in the gas, and the second one is the heterogeneous reaction on the particle surface. The reaction rate in the gas is determined by the second-order kinetics (the first-order kinetics for methane and the first-order kinetics for oxygen). The specific reaction rate of the gas depends on the temperature under the Arrhenius law. The heterogeneous reaction rate is limited by the mass-transfer coefficient β. The friction between the particles and the gas is taken into account.

The mathematical model is based on the dual-velocity two-phase model of the reacting gas-dispersion medium. The system of equations includes the mass-conversation equation, the impulse-conversation equation, the total energy-conversation equation of the gas and the particles taking into account the thermal conductivity and the chemical reactions in the gas and on the particle surface, the mass-conversation equation of the mixture gas components considering the diffusion and the combustion and the particle radius and concentration equations. The mathematical formulation of the problem under the made assumptions has the following form:

The gas continuity equation:

$$\frac{\partial \rho_g}{\partial t}+\frac{\partial \rho_g u_g}{\partial r}=-\frac{2\rho_g u_g}{r}+G. \tag{1}$$

The gas impulse–conversation equation:

$$\frac{\partial\left(\rho_g u_g\right)}{\partial t}+\frac{\partial\left(\rho_g u_g^2+p\right)}{\partial r}=-\frac{2\rho_g u_g^2}{r}-\tau_{tr}+Gu_k. \tag{2}$$

The gas energy-conversation equation:

$$\begin{gathered}\frac{\partial \rho_g\left(\varepsilon_g+\frac{u_g^2}{2}\right)}{\partial t}+\frac{\partial\left[\rho_g u_g\left(\varepsilon_g+\frac{u_g^2}{2}\right)+pu_g\right]}{\partial r}=-\frac{2\left[\rho_g u_g\left(\varepsilon_g+\frac{u_g^2}{2}\right)+pu_g\right]}{r}+Gc_{p,k}T_k-u_k\tau_{tr}+\\ G\frac{u_k^2}{2}+\alpha_k n_k S_k\left(T_k-T_g\right)+\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\lambda\left(T_g\right)\frac{\partial T_g}{\partial r}\right)+Q_1 k_{01}\rho_{CH4}\rho_{O2}\exp\left(-\frac{E_1}{R_u T_g}\right).\end{gathered} \tag{3}$$

The methane mass balance equation:

$$\frac{\partial \rho_{CH4}}{\partial t}+\frac{\partial \rho_{CH4}u_g}{\partial r}=-\frac{2\rho_{CH4}u_g}{r}+\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D\left(T_g\right)\frac{\partial \rho_{CH4}}{\partial r}\right)-k_{01}\rho_{CH4}\rho_{O2}\exp\left(-\frac{E_1}{R_u T_g}\right). \tag{4}$$

The oxygen mass balance equation:

$$\frac{\partial\rho_{O2}}{\partial t}+\frac{\partial\rho_{O2}u_g}{\partial r}=-\frac{2\rho_{O2}u_g}{r}+\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2D\left(T_g\right)\frac{\partial\rho_{O2}}{\partial r}\right)-\alpha_1G-\alpha_2k_{01}\rho_{CH4}\rho_{O2}\exp\left(-\frac{E_1}{R_uT_g}\right). \quad (5)$$

The particle mass balance equation:

$$\frac{\partial\rho_k}{\partial t}+\frac{\partial\rho_ku_k}{\partial r}=-\frac{2\rho_ku_k}{r}-G. \quad (6)$$

The particle impulse–conversation equation:

$$\frac{\partial\left(\rho_k u_k\right)}{\partial t}+\frac{\partial\rho_ku_k^2}{\partial r}=-\frac{2\rho_ku_k^2}{r}+\tau_{tr}-Gu_k. \quad (7)$$

The particle energy-conversation equation:

$$\frac{\partial\rho_k\left(\varepsilon_k+\frac{u_k^2}{2}\right)}{\partial t}+\frac{\partial\rho_ku_k\left(\varepsilon_k+\frac{u_k^2}{2}\right)}{\partial r}=-\frac{2\rho_ku_k\left(\varepsilon_k+\frac{u_k^2}{2}\right)}{r}-\alpha_k S_kn_k\left(T_k-T_g\right)+Q_2G-Gc_{p,k}T- \quad (8)$$
$$G\frac{u_k^2}{2}+\tau_{tr}u_k.$$

The particle number concentration equation:

$$\frac{\partial n_k}{\partial t}+\frac{\partial n_k u_k}{\partial r}=-\frac{2n_k u_k}{r}. \quad (9)$$

The particle radius equation:

$$r_k=\left(\frac{3\rho_k}{4\pi\rho_k^0 n_k}\right)^{1/3}. \quad (10)$$

The perfect-gas law:

$$p=\rho_gR_gT_g. \quad (11)$$

The particle temperature equation:

$$T_k=\frac{\varepsilon_k}{c_k}. \quad (12)$$

The initial condition:

$$T_g\left(r,0\right)=\begin{cases}T_z,\ 0\le r\le r_0\\ T_b,\ r_0<r\le r_s\end{cases},\ T_k\left(r,0\right)=T_b,\ \rho_{CH4}\left(r,0\right)=\rho_{CH4,b},\ \rho_{O2}\left(r,0\right)=\rho_{O2,b}, . \quad (13)$$
$$\rho_k\left(r,0\right)=\rho_{k,b},\ u_g\left(r,0\right)=u_k\left(r,0\right)=0,\ p\left(r,0\right)=p_b,\ n_k\left(r,0\right)=n_{k,b}.$$

The boundary conditions:

$$\frac{\partial\rho_{CH4}\left(0,t\right)}{\partial r}=\frac{\partial\rho_{O2}\left(0,t\right)}{\partial r}=\frac{\partial T_g\left(0,t\right)}{\partial r}=0,\ u_k\left(0,t\right)=u_g\left(0,t\right)=0. \quad (14)$$

$$\frac{\partial\rho_{CH4}\left(r_S,t\right)}{\partial r}=\frac{\partial\rho_{O2}\left(r_S,t\right)}{\partial r}=\frac{\partial T_g\left(r_S,t\right)}{\partial r}=0,\ u_k\left(r_S,t\right)=u_g\left(r_S,t\right)=0. \quad (15)$$

Where : $\varepsilon_g=\dfrac{p}{\rho_g\left(\gamma-1\right)}$ – the internal gas energy, $\varepsilon_k=c_kT_k$ – the internal particle energy, $\lambda=\lambda_{st}\left(\dfrac{T}{T_v}\right)^s$ – the thermal conductivity [8], $D=D_{st}\left(\dfrac{T}{T_v}\right)^s$ – the diffusion coefficient, $\alpha_k=\dfrac{Nu_k\lambda_g}{2r_k}$ – the gas-particles heat transfer coefficient, $\gamma=\dfrac{c_p}{c_v}$ – the adiabatic exponent, $\beta_{m,i}=\dfrac{\lambda_g\left(T\right)Nu_D}{c_g\rho_gr_{k,i}}$ – – the particles mass-transfer coefficient [10], $G=\alpha_5n_kS_kj_1\rho_{O2}$ – the rate of mass changing,

$j_1 = \dfrac{\beta_m k_{02} \exp\left(-E_2/R_u T_k\right)}{\beta_m + k_{02} \exp\left(-E_2/R_u T_k\right)}$ – the heterogeneous reaction rate, $\tau_{tr} = n_k F_{tr}$, – the gas-particles interacting force, $F_{tr} = \dfrac{12\left(1+0.15\,\mathrm{Re}^{0.682}\right) S_m\, \rho_g\left(u_g - u_k\right)\left|u_g - u_k\right|}{\mathrm{Re}}$, $\mathrm{Re} = \dfrac{2\rho_g r_k \left|u_g - u_{k,i}\right|}{\eta}$ – Reynolds number, $Nu_k = 2 + \left(Nu_l^2 + Nu_t^2\right)^{1/2}$, $Nu_l = 0.664\,\mathrm{Re}^{0.5}$, $Nu_t = 0.037\,\mathrm{Re}^{0.8}$, $\alpha_1 = \dfrac{\mu_{O2}\nu_{O2}}{\mu_C \nu_C}$ – stoichiometric coefficient in coal-oxygen reaction, $\alpha_2 = \dfrac{\mu_{O2}\nu_{O2}}{\mu_{CH4}\nu_{CH4}}$ – stoichiometric coefficient in methane-oxygen reaction, , ρ – the density, ρ_{CH4} – the methane partial density, ρ_{O2} – the oxygen partial density, *u* – the velocity, *t* – the time, *r* – the radius coordinate, r_k – the particle radius, *p* – the pressure, λ – the thermal conductivity, *D* – the diffusion coefficient, *Q* – the reaction heat, k_0 – pre-exponential factor in the Arrhenius law, *T* – the temperature, *E* – energy of activation, R_u – the molar gas constant, R_g – gas constant, r_0 – the radius of the high-temperature region (the hot spot), r_S – the radius of the spherical volume. Indexes: *b* – the initial conditions of the methane-air mixture state parameters, *g* – gas parameters; *k* – particle parameters. For *Q*, k_0, *E* index 1 is the parameters of the reaction in the gas; index 2 is the parameters of the heterogeneous reaction.

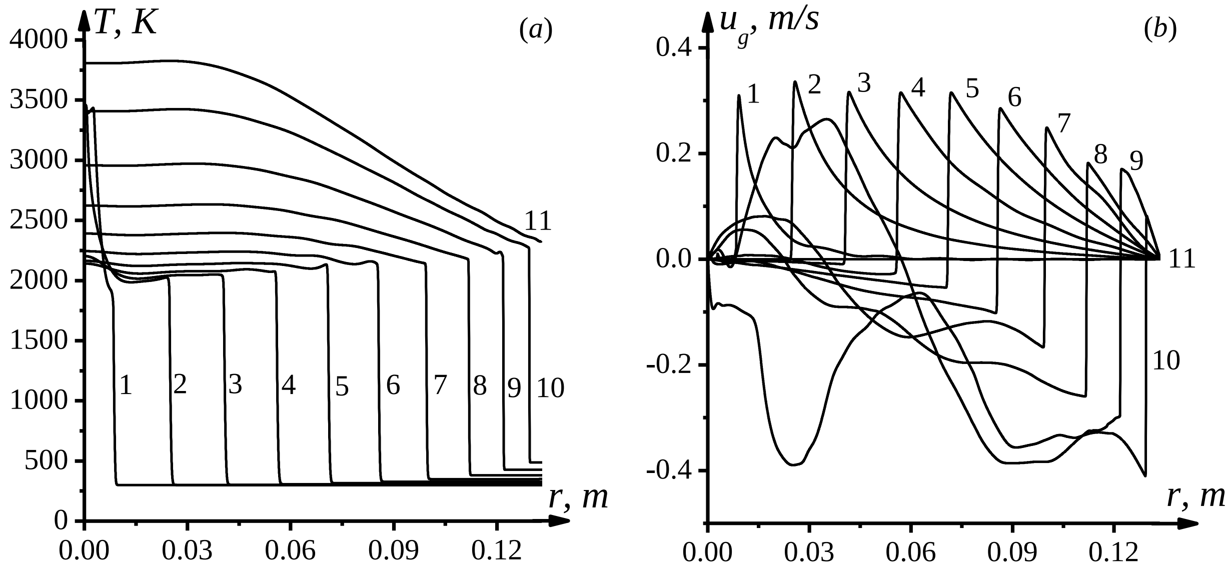
The problem (1) – (15) was solved numerically by S.K. Goduvov's method [11]. The summands on the right side of equations which determine the diffusion and the heat transfer processes were explicit approximated by the three-point stencil. To solve the equations (1) – (5) the breakdown breakup of an arbitrary discontinuity scheme of gas parameters was used [11]. To solve the equations (6) – (8) the method from [12] was used. The spatial step was set to $\Delta h = 10^{-5}$ *m* to provide the sufficient number of different scheme points in the region of the reaction and warm-up zone in front of the burning front. The value of the step provides at least 30 points of difference scheme in the warm-up zone. The time step was calculated by Courant's stability criterion $\Delta t = \dfrac{0.8\Delta h}{\max\left[c\right] + \max\left[\left|u\right|\right]}$, where *c* is the sound velocity.

To verify the computer program the test problem about the thermal explosion in an enclosed volume has been solved. The determination error of the adiabatic temperature after the explosion was equal to 1 %. The value of the hot spot energy was larger than the critical ignition energy of the mixture.

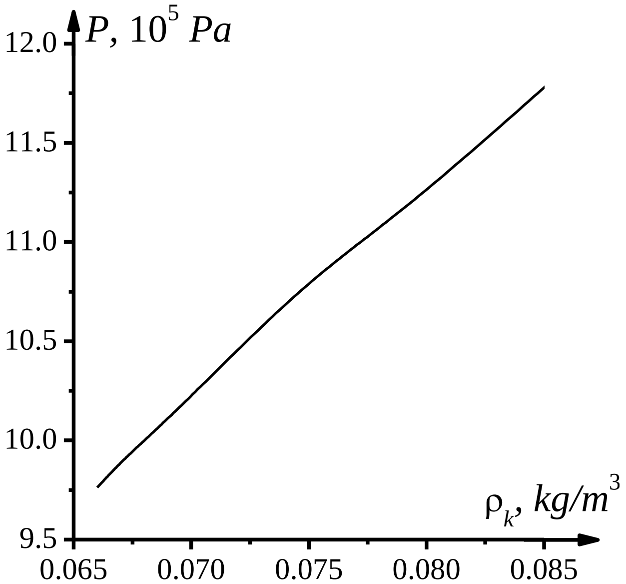
3. Results and discussion

The calculations were held under the following parameters: $Q_1 = 55.7$ *MJ/kg*, $Q_2 = 29$ *MJ/kg*, $k_{01} = 1.125\cdot10^{12}$ $m^3/(kg\cdot s)$, $k_{02} = 7.9\cdot10^4$ *m/s*, $E_1 = 239$ *kJ/mol*, $E_2 = 135$ *kJ/mol*, $c_{p,g} = 1065$ *J*/(*kg*·*K*), $c_{v,g} = 768.2$ *J*/(*kg*·*K*), $c_k = 1464.4$ *J*/(*kg*·*K*), $\rho_k^0 = 1400\ kg/m^3$, $\rho_{CH4,b} = 6.4\cdot10^{-3}\ kg/m^3$, $\rho_{O2,b} = 0.264\ kg/m^3$, $\lambda_{st} = 0.025$ *W*/(*m*·*K*), $\eta = 2\cdot10^{-5}$ *Pa*·*s*, $D_{st} = 1.992\cdot10^{-5}$ m^2/s, $p_b = 0.1$ *MPa*, *s* = 2/3, $R_u = 8.31$ *J*/(*mol*·*K*), $R_g = 288.95$ *J*/(*kg*·*K*), $\alpha_1 = 2.67$, $\alpha_2 = 4$, γ = 1.39, $r_0 = 2\cdot10^{-3}$ *m*, $T_b = 300$ *K*, $V = 10^{-2}$ m^3, $r_s = 0.134$ *m*, $r_{k,b} = 10^{-6}$ *m*, $T_z = 1500$ *K*. The value of particle density ρ_k was varied in the range of 0.065 ÷ 0.085 kg/m^3. The results of the calculations are shown in Pic. 1 – 3.

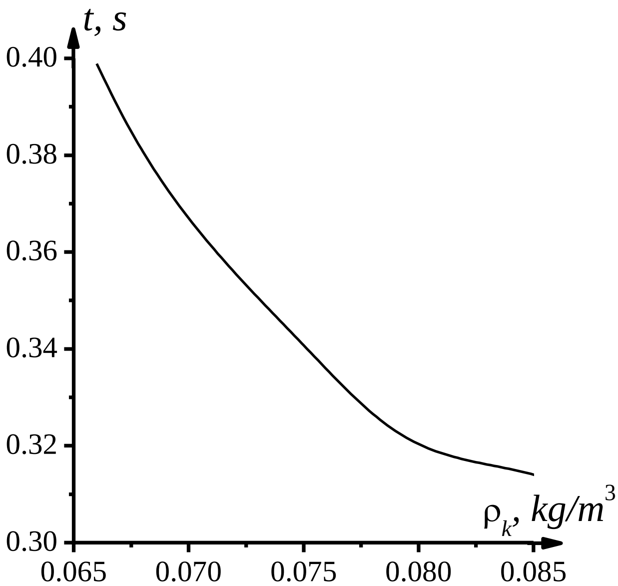
The distribution of the temperature and the gas velocity at different moments of time under coal particle mass $\rho_{k,b} = 0.068$ kg/m^3 are shown in Pic 1. The curves 11 correspond to the state of the temperature and the gas velocity after the burn out of the whole mixture in the volume. It has been determined from the calculations that the particle velocity was almost the same as gas velocity. We have obtained the pressure-coal particle mass curve (Pic. 2) and the time-coal particle mass curve (Pic. 3) at the end of the burning. The increase of the coal particle mass leads to the increase of the pressure in the volume (Pic. 2) and to the decrease of the mixture total burn out time (Pic. 3).



Pic. 1. The temperature distributions (*a*) and the gas velocity distributions (*b*) at the fixed moments of the time. $\rho_{k,b}$ = 0.068 kg/m^3; $r_{k,b} = 10^{-6}$ m; 1 – t = 0.02 s, 2 – t = 0.06 s, 3 – t = 0.1 s, 4 – t = 0.14 s, 5 – t = 0.18 s, 6 – t = 0.22 s, 7 – t = 0.26 s, 8 – t = 0.3 s, 9 – t = 0.34 s, 10 – t = 0.38 s, 11 – t = 1 s



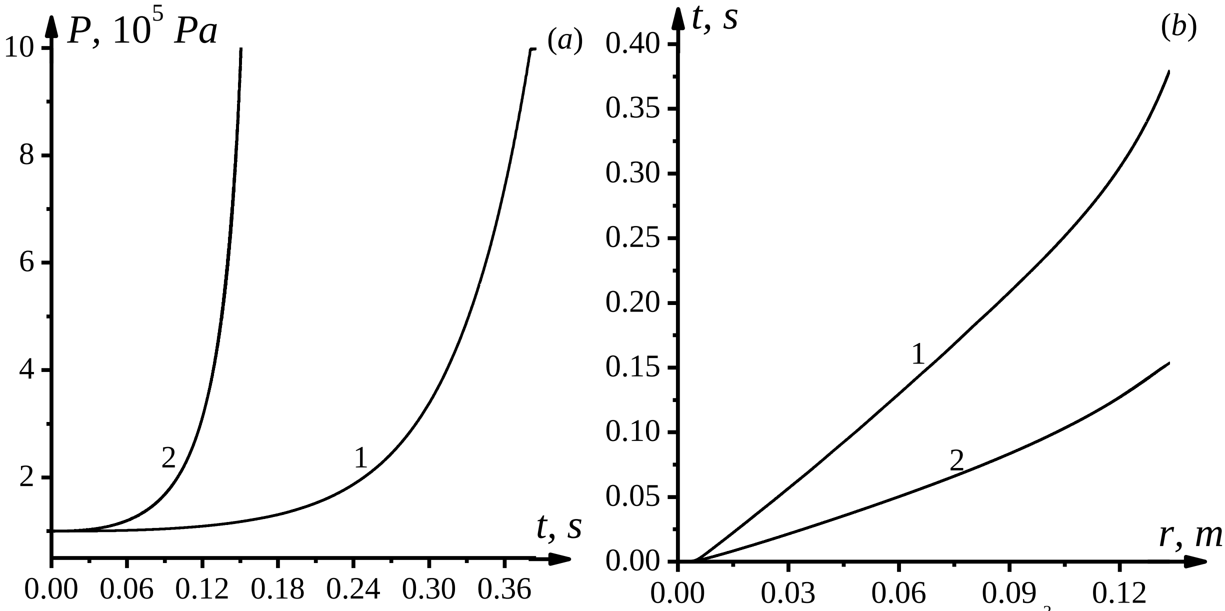
Pic. 2. The pressure-coal particle mass curve at the end of the burning



Pic. 3. The time-coal particle mass curve at the end of the burning

The hot spot ignites the mixture in the center of the volume. The amount of the methane in the mixture is not enough to support the burning therefore the flame front propagation depends on the amount of the coal dust in the volume. According to the obtained results the flame front doesn't propagate along the volume when the coal dust mass is less than 0.065 kg/m^3 and the particle size is more than $r_{k,b} = 10^{-6}$ m. The particles don't have enough time to react and the burning is extinguished. But if the particle size is less than $r_{k,b} = 10^{-7}$ m and the coal dust mass is less than 0.065 kg/m^3 the burning of the coal dust methane-air mixture becomes possible. It is largely due to the quick burning of the small particles which are able to support the burning front.

Pic. 4*a* shows the pressure growth-time curves under ρ_k = 0.068 kg/m^3. Pic. 4*b* shows the curves of the flame front propagation in time. The flame front coordinate is r in which the content of the oxidizer is half of the initial value. The rate of the pressure growth increases with the decrease of the coal particles size (Pic. 4*a*).



Pic. 4. The pressure change in time (*a*), flame front coordinate (*b*). ρ_k = 0.068 kg/m^3;
$r_{k,b}$ = 10^{-6} *m* (curve 1), 10^{-7} *m* (curve 2)

4. Conclusions

We have carried out the numerical simulation of the coal dust methane-air mixture flame propagation in the enclosed spherical volume with the hot spot in the center. The influence of the coal particle mass on the pressure in the volume after the mixture burn-out and on the burn-out time has been investigated. We have obtained the pressure growth rate-coal particle size dependences.

Acknowledgments

This work was supported by the Russian Science Foundation grant No. 16-33-60091 mol_a_dk.

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