The burning rate of coal-dust-air suspension

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Abstract. The paper provides the numerical investigation on the propagation of the coal dust-air combustion front. We determined the apparent and normal burning rate of the coal dust-air suspension depending on the size and mass concentration of coal dust and on the percentage of volatile components in coal dust particles. We also made an analysis on the influence of the percentage content of volatile components on the burning rate of the suspension with small and large particle radiiuses.

1. Introduction
The paper is devoted to the problem of propagation of the coal dust-air combustion front. According to the results of experimental studies available in the scientific literature, the combustion front propagation velocity of a hybrid gas suspension is significantly influenced by the composition of the gas suspension: the size and mass concentration of coal dust particles, the percentage of volatile components in the particles and the mass content of the combustible components in the gas.

In this paper we numerically investigate the problem of the combustion front propagation velocity on the basis of approaches and results [1 – 3] and using the experimental research [4] to verify the obtained simulation data. The aim of the study is to determine the influence of the suspension composition (the size and mass concentration of dust particles and the volatile components) on the propagation velocity of the combustion front.

2. Mathematical model
The physico-mathematical formulation of the problem is based on the approaches from papers [1 – 3]. The coal dust is assumed to be uniformly distributed in the air. The volume fraction of the particles is low, the mass concentration of the particles $p_{db}$, the particle size $r_k$ and the volatile components $V^c$. There is an ignition spot with thickness $x_0$ on the left border of the calculation area. The diffusion and thermal conductivity coefficients of the gas depend on temperature. A heterogeneous first-order oxygen reaction occurs on the surface of the particles. The rate of the reaction is described taking mass transfer into account. The liberation of volatile components from the particles is set by a first-order reaction according to the Arrhenius law. The released volatiles pass into the gas and are capable to react with the oxidizer. The rate of the homogeneous reaction between gaseous volatiles and oxygen is determined by the second-order reaction according to the Arrhenius law (the first-order for oxygen and for the combustible). The thermal and dynamic interaction between particles and gas is taken into account. The mathematical formulation of the problem under the made assumptions is well fitted by a system of equations written in a Cartesian coordinate system.
\[ \frac{\partial \rho_s}{\partial t} + \frac{\partial \rho_s u_s}{\partial x} = G_2 + G_3, \]  
(1)

\[ \frac{\partial (\rho_s u_s)}{\partial t} + \frac{\partial (\rho_s u_s^2 + p)}{\partial x} = -\tau_v + (G_2 + G_3)u_k, \]  
(2)

\[ \frac{\partial \rho_s (e_s + 0.5u_s^2)}{\partial t} + \frac{\partial \left[ \rho_s u_s (e_s + 0.5u_s^2) + pu_s \right]}{\partial x} = \frac{\partial}{\partial x} \left( \lambda_s \frac{\partial T_s}{\partial x} \right) - u_k \tau_v + \left( G_2 + G_3 \right) \left( \frac{u_k^2}{2} + c_k T_k \right) + \alpha_k n_k S_k \left( T_k - T_s \right) + Q_k \rho_0 T_0 \rho_{02} \exp \left( \frac{-E_1}{R_k T_k} \right), \]  
(3)

\[ \frac{\partial \rho_{02}}{\partial t} + \frac{\partial \rho_{02} u_s}{\partial x} = \frac{\partial}{\partial x} \left( \rho_s D_s (T_s) \frac{\partial a_{02}}{\partial x} \right) - \alpha_2 G_2 - \alpha_1 \rho_0 \rho_{02} \exp \left( \frac{-E_1}{R_k T_k} \right), \]  
(4)

\[ \frac{\partial \rho_o}{\partial t} + \frac{\partial \rho_o u_s}{\partial x} = \frac{\partial}{\partial x} \left( \rho_s D_s (T_s) \frac{\partial a_o}{\partial x} \right) - \alpha_0 \rho_0 \rho_{02} \exp \left( \frac{-E_1}{R_k T_k} \right) + G_5, \]  
(5)

\[ \frac{\partial \rho_l}{\partial t} + \frac{\partial \rho_l u_k}{\partial x} = -G_3, \]  
(6)

\[ \frac{\partial \rho_s}{\partial t} + \frac{\partial \rho_s u_k}{\partial x} = - (G_2 + G_3), \]  
(7)

\[ \frac{\partial (\rho_s u_k)}{\partial t} + \frac{\partial (\rho_s u_k^2)}{\partial r} = \tau_v - (G_2 + G_3)u_k, \]  
(8)

\[ \frac{\partial \rho_s (e_s + 0.5u_s^2)}{\partial t} + \frac{\partial \rho_s u_k (e_s + 0.5u_s^2)}{\partial r} = -\alpha_1 n_k S_k \left( T_k - T_s \right) + Q_2 G_2 - Q_3 G_3 - c_k T_k \left( G_2 + G_3 \right) - \left( G_2 + G_3 \right) \frac{u_k^2}{2} + \tau_v u_k, \]  
(9)

\[ \frac{\partial n_k}{\partial t} + \frac{\partial n_k u_k}{\partial r} = 0, \]  
(10)

\[ T_s \left( x, t \right) = \begin{cases} T_0, & 0 \leq x \leq x_0, \\ T_b, & x_0 < x < \infty \end{cases}, \]  
(12)

\[ \rho_{02} \left( x, t \right) = 0, \rho_s \left( x, t \right) = \rho_{02} u_{02}, \rho_s \left( x, t \right) = u_k \left( x, t \right) = 0, n_k \left( x, t \right) = n_{0k}, \]  
(13)
The following notations are used in (1) – (13): \( \rho_g \) is the gas density; \( \rho_i \) is the distributed particle mass per unit volume; \( \rho_{O_2} \) is the distributed volatile mass in particles per unit volume; \( \rho_{gl} \) is the partial volatile density in the gas; \( \rho_{O_2} \) is the oxygen partial density; \( a_{O_2} \ a_{gl} \) is the mass concentrations of oxygen and volatiles; \( u \) is the velocity; \( t \) is the time; \( x \) is the coordinate; \( p \) is the pressure; \( r_i = \left( 3 \left( \rho_i - \rho_g \right) / 4 \pi n_i \rho_i ^0 \left( 1 - V_C \right) \right) ^ {1/3} \) is the particle radius; \( Q \) is the reaction heat; \( k_0 \) is the constant of the chemical reaction rate; \( T \) is the temperature; \( E \) is the energy of activation; \( R_o \) is the mol gas constant; \( c_p \) is the gas heat capacity at constant pressure; \( c_v \) is the gas heat capacity at constant volume; \( c_k \) is the gas heat capacity of the coal particles; \( \epsilon_k = c_k T_k \) is the particle internal energy; \( \varepsilon_g = p / \rho_g \left( \gamma - 1 \right) \) is the gas internal energy; \( \lambda_x = \lambda _{av} \left( T_g / T_r \right) ^{3/2} \) is the gas thermal conductivity coefficient; \( D_k \) is the gas diffusion coefficient; \( \alpha_k = N u_k \lambda_x / 2r_i \) is the gas-particles heat exchange coefficient; \( \alpha_k = \mu_{O_2} \nu_{O_2} / \mu_g \nu_{gl} \), \( \alpha_s = \mu_{O_2} \nu_{O_2} / \mu_v \nu_v \) is the oxygen consumption coefficient in reaction with volatile and coal particle respectively; \( \mu_{O_2}, \mu_{gl}, \mu_v \) is the molar masses of oxygen, volatiles and carbon; \( \nu_{O_2}, \nu_{gl}, \nu_v \) is the reaction stoichiometric coefficients; \( \gamma = c_p / c_v \) is the adiabatic exponent; \( \chi_x = \lambda_x / \left( c_v \rho_g \right) \) is the heat diffusivity; \( V_C \) is the percentage of volatiles in the particle. Indexes: \( b \) - the initial conditions of the state parameters, \( k \) – the particle parameters, \( g \) – the gas parameters, index 1 is for kinetics parameters of the homogeneous reaction in the gas; index 2 - for the heterogeneous reaction on the particle surface, index 3 - for the gasification reaction of volatile components.

The rate of particle mass change during its combustion is determined from the equation:

\[
G_2 = n_k \rho_{O_2} \beta_{O_2} k_{O_2} e^{-E_i / R_T} \left[ \beta_m + k_{O_2} e^{-E_i / R_T} \right] \left( \beta_m + k_{O_2} e^{-E_i / R_T} \right),
\]

where \( \beta_m = \lambda_x \left( T \right) N u_d / \rho_g, \rho_g \) is the particles mass-transfer coefficient. The rate of particle mass change during gasification is

\[
G_3 = \rho_i k_{O_2} e^{-E_i / R_T}.
\]

The friction force is defined by

\[
\tau _n = n_k F_n, \quad \left[ \frac{\rho_g - \rho_i}{\eta} \right] \left| u_g - u_i \right| / 2 \text{ is the interaction force of a single particle with the gas,}
\]

\[
C_r = 24 \left( 1 + 0.15 \text{Re}^{0.62} \right) / \text{Re} \text{ is the friction coefficient,}
\]

\[
\text{Re} = 2 \rho_i / \left| u_g - u_i \right| / \eta \text{ is the Reynolds number,} \quad \text{Nu}_d = 2 + \left( \text{Nu}_d^2 + \text{Nu}_d^2 \right) ^{1/2} \text{ is the Nusselt number,}
\]

\[
\text{Nu}_d = 0.664 \sqrt{\text{Re}}, \quad \text{Nu}_i = 0.037 \text{Re}^{0.8}, \text{ S}_m \text{ is the cross-sectional area,} \quad \eta \text{ is the gas coefficient of dynamic viscosity.}
\]

The methodology of the numerical solution was described in detail in [3], where the authors used method of S.K. Godunov [5] and the algorithm [6] to solve the problem of the critical conditions for spark ignition of a coal dust-air suspension. In this paper, we numerically investigate the problem of the burning rate of a coal dust-air suspension. The initial condition concerning the ignition spot was set specifically to provide on the one hand the sufficient energy to ignite the suspension, on the other hand, not to insert a large amount of thermal energy into the dust cloud.

### 3. Results and discussion

The calculations were held for the particle radius range \( r_i = 5 \cdot 10^{-7} \div 2 \cdot 10^{-6} \text{ m} \), the particle mass concentration \( \rho_{kh} = 0.12 \div 0.4 \text{ kg/m}^3 \) and the percentage of the volatile components \( V_C = 0.1 \div 0.4 \). The selected mass concentration of coal dust corresponds to combustion in a lack of oxidant. Other thermophysical and kinetic parameters of coal dust were: \( Q_1 = 20 \text{ MJ/kg,} \quad k_0 = 1214.3 \text{ m}^3/(\text{kg·s}), \quad E_1 = 55.3 \text{ kJ/mol,} \quad \alpha_1 = 3.5, \quad k_{O_2} = 79 \cdot 10^3 \text{ m/s,} \quad E_2 = 135 \text{ kJ/mol,} \quad Q_2 = 20 \text{ MJ/kg,} \quad \alpha_2 = 2.67, \quad k_0 = 5.83 \cdot 10^{15} \text{ s}^{-1}, \quad E_3 = 209 \text{ KJ/mol,} \quad Q_3 = 0.18 \text{ MJ/kg,} \quad R_o = 8.31 \text{ J/(mol·K),} \quad c_{p,x} = 1065 \text{ J/(kg·K),} \quad c_{v,x} = 768.2 \text{ J/(kg·K),} \quad \lambda_0 = 0.025 \text{ W/(m·K),} \quad c_k = 1464.4 \text{ J/(kg·K),} \quad T_b = 300 \text{ K,} \quad \rho_i^0 = 1400 \text{ kg/m}^3, \quad \eta = 2 \cdot 10^{-5} \text{ Pa·s,} \quad D_n = 1.992 \cdot 10^{-5} \text{ m}^2/s, \quad \rho_{O_2,h} = 0.264 \text{ kg/m}^3, \quad p_0 = 0.1 \text{ MPa.}
The process of particle heating and igniting proceeds in the following way. At the initial time the gas heats particles in the region of the ignition spot. At a particle temperature of 500-550 K, the volatile components from the particles begin to release into the gas. The post-heating of the gas leads to the onset of chemical reactions in the gas. The chemical reactions provide further heating of the gas suspension and a heterogeneous chemical reaction occurs on the particles. The reaction on the particles leads to the subsequent propagation of the combustion front along the gas suspension. The velocity of flame propagation depends on the content of volatile components in the particles, the size and the mass concentration of the particles.

Each numerical simulation with different composition of the mixture (radius and mass concentration of particles, and the percentage of volatiles) continued until the steady flame propagation regime was established. The apparent velocity of the combustion front was determined from the coordinate $x$, where the partial density of the oxidizer was equal to 0.01 of the initial value. The normal burning rate was determined as the difference between the apparent burning rate of the suspension and the velocity of the gas motion. Examples of the results obtained are shown in Figures 1 – 4.

Figure 1 shows the dependence of the normal burning rate of the suspension on the mass concentration of particles with the radius 1 $\mu$m. The curves correspond to the calculations for coal dust with the content of volatile components 0.1, 0.2, 0.3. Figure 2 presents the calculated apparent burning rate of a coal dust suspension with the same composition as in Figure 1. An increase in the percentage of volatile components leads to a decrease in the apparent and normal propagation velocity of the combustion front for particle radius 1 $\mu$m.

The dependence of the apparent burning rate of the suspension on the particle radius for the percentage of volatile components 0.1 and 0.3, respectively are presented in Figures 3 – 4. The curves correspond to the calculations for the air suspension with coal dust mass concentration of 0.15, 0.3, 0.4 $kg/m^3$. The suspension with the mass concentration of 0.3 $kg/m^3$ has the greatest dependence of the burning rate on the percentage of volatile components in the particles.
The numerical simulation shows that the burning rate of the small particles with a radius of 0.5 μm is practically independent of the content of the volatile components in the particles. The small particles heat up more quickly and reactions on particles and in the gas proceed almost simultaneously. For the large particles the content of volatile components plays an important role, since the heating time of the particles is greater. As can be seen from Figures 3 – 4 for a mass concentration of coal dust over 0.3, the apparent burning rate of the coal dust-air suspension varies slightly with the change in particle size and has a weak dependence on the percentage of volatile components in the particles. This is due to the fact that at high mass concentrations of coal dust combustion takes place with a significant lack of the oxidant. In this case, there is not complete burn-out of the particles and the evolved gaseous volatile components.

4. Conclusions
We have numerically investigated the dependence of the coal dust-air suspension combustion rate on the radius and mass concentration of coal dust particles and on the percentage of volatile components in the particles. It has been shown that fine particles burn with a higher rate, which practically does not depend on the particle radius. While as for large particles the percentage of volatile components in the particles influences on the apparent burning rate. Moreover the apparent burning rate is low at high mass concentrations of coal dust in the suspension.

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