Numerical determination of the combustion rate of a gas suspension of coal dust in a propane-air mixture

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Abstract. The results of the numerical solution of the problem of the combustion rate of a coal-propane-air mixture are presented. The physical and mathematical formulation of the problem is based on the approaches of the dynamics of multiphase reacting media. The method for solving the problem is based on the algorithm for the decay of an arbitrary discontinuity. The dependences of the visible and normal combustion rate of the coal-propane-air mixture on the radius and the volumetric content of propane in the gas are obtained.

1. Introduction
Suspended organic dust is a potentially dangerous ignition source. Separately, combustible gas and organic dust can be difficult to ignite, while their mixture can be a highly flammable compound that burns at a relatively high speed.

Earlier, a physical and mathematical model of ignition and combustion of a propane-air mixture was proposed [1]. The effective constants in the law of the combustion rate of the propane-air mixture were determined, and good agreement of the obtained results of the calculated combustion rate of the mixture with the data from the scientific literature was shown.

In this work, the aim is to determine the combustion rate of a propane-air mixture with an admixture of coal dust.

2. Mathematical model
The physical and mathematical formulation of the problem is formulated under the following assumptions. It is assumed that a suspension of coal dust with a total mass concentration \( m_{\text{dust}} \) of particles, with particle size being denoted as \( r_p \), is uniformly distributed in the propane-air mixture. It is assumed that the volume fraction of particles is small. Gas diffusion and thermal conductivity coefficients depend on temperature. Thermal and dynamic interactions between particles and gas are taken into account. On the surface of the particles, a heterogeneous reaction of the first order with respect to oxygen occurs. The rate of a heterogeneous chemical reaction on particles is described taking into account mass transfer. In the gas, chemical reactions take place between the combustible component of the feed gas (propane) and the oxidizing agent.

Other assumptions of the mathematical combustion model correspond to [1, 2] and the model has the following form:

the gas continuity equation:

\[
\frac{\partial \rho_g}{\partial t} + \frac{\partial \rho_g u}{\partial x} = G_2, \tag{1}
\]
the momentum conservation equation for the gas

$$\frac{\partial \rho_g u_g}{\partial t} + \frac{\partial (\rho_g u_g^2 + p_g)}{\partial x} = -\tau_g + G_2 u_p, \quad (2)$$

the gas energy equation:

$$\frac{\partial \rho_g (\varepsilon_g + 0.5u_g^2)}{\partial t} + \frac{\partial [\rho_g u_g (\varepsilon_g + 0.5u_g^2) + pu_g]}{\partial x} = \frac{\partial}{\partial x} \left( \eta_g \frac{\partial T_g}{\partial x} \right) + QG_t + G_2 \left( 0.5u_p^2 + c_p T_p \right) - u_p \tau_p + \alpha_p n_p S_p \left( T_p - T_g \right), \quad (3)$$

do the oxygen mass balance equation:

$$\frac{\partial \rho_{ox}}{\partial t} + \frac{\partial \rho_{ox} u_{ox}}{\partial x} = \frac{\partial}{\partial x} \left( \rho_{ox} D_{ox} \frac{\partial a_{ox}}{\partial x} \right) - \alpha_s G_t - \alpha_s G_2, \quad (4)$$

the balance equation for the mass of the combustible component in the gas:

$$\frac{\partial \rho_f}{\partial t} + \frac{\partial \rho_f u_f}{\partial x} = \frac{\partial}{\partial x} \left( \rho_f D_f \frac{\partial a_f}{\partial x} \right) - G_t, \quad (5)$$

the particle mass balance equation:

$$\frac{\partial \rho_p}{\partial t} + \frac{\partial \rho_p u_p}{\partial x} = -G_2, \quad (6)$$

the particle momentum conservation equations

$$\frac{\partial (\rho_p u_p)}{\partial t} + \frac{\partial \rho_p u_p^2}{\partial x} = \tau_p - G_2 u_p, \quad (7)$$

the particle energy equations:

$$\frac{\partial \rho_p (\varepsilon_p + 0.5u_p^2)}{\partial t} + \frac{\partial \rho_p u_p (\varepsilon_p + 0.5u_p^2)}{\partial x} = QG_2 - \alpha_p S_p n_p \left( T_p - T_g \right) - G_2 \left( c_p T_p + 0.5u_p^2 \right) + \tau_p u_p, \quad (8)$$

the particle concentration equation:

$$\frac{\partial n_p}{\partial t} + \frac{\partial n_p u_p}{\partial x} = 0, \quad (9)$$

the gas equation:

$$p_g = \rho_g R_g T_g, \quad (10)$$

the initial conditions:

$$T_g (x,0) = \begin{cases} T_0, & 0 \leq x \leq x_0 \\ T_{gb}, & x_0 < x \leq \infty \end{cases}, \quad T_{gb}, \quad p_g (x,0) = p_{gb},$$

$$\rho_m (x,0) = \rho_{m,b}, \quad u_g (x,0) = u_p (x,0) = 0, \quad \rho_p (x,0) = m_{dust}, \quad n_p (x,0) = n_{p,b}. \quad (11)$$
the boundary conditions:
\[
\frac{\partial \rho_p (0,t)}{\partial x} = \frac{\partial \rho_{ox} (0,t)}{\partial x} = \frac{\partial n_p (0,t)}{\partial x} = \frac{\partial T_p (0,t)}{\partial x} = \frac{\partial T_{ox} (0,t)}{\partial x} = 0,
\]
\[
\frac{\partial \rho_{ox} (\infty,t)}{\partial x} = \frac{\partial T_{ox} (\infty,t)}{\partial x} = 0, u_p (0,t) = u_{ox} (0,t) = 0.
\]

The main notations in (1) - (12) are usual and correspond to the studies [3 – 4]. In equations (3) and (10) \( \varepsilon \) is the internal energy, which for a gas is determined by the equation \( \varepsilon_p = p_p/(\rho_p (\gamma - 1)) \), where \( \gamma = c_p/c_v \) is the adiabatic exponent; and for particles, the internal energy is defined as \( \varepsilon_p = c_p T_p \). The coefficients \( \alpha_1 = \mu_{a,v_{ox}}/(\mu_{j,v_f}) \) and \( \alpha_2 = \mu_{a,v_{ox}}/(\mu_{c,v_c}) \), determine the oxygen consumption in reactions with coal dust particles released by the volatile and combustible components in the gas, respectively. The notations are \( \mu_{a,v}, \mu_{c,v} \) - the molar masses of the oxidizer, carbon and the combustible gas component, and \( v_{ox}, v_c, v_f \) - the stoichiometric reaction coefficients.

The rate of the chemical reaction in the gas between the reactive components of the feed gas and the oxidant is determined from the equation:
\[
G_1 = \rho_f \rho_{ox} k_{ox} \exp \left(-E_{a,4}/(R_T)\right),
\]
where \( \rho_f \) is the partial density of the combustible component of the source gas.

The rate of chemical reaction on the surface of the particles is defined as:
\[
G_2 = n_p S_p j_2 \rho_{ox},
\]
where \( j_2 = \beta_n k_{ox} \exp \left(-E_{a,2}/(R_T)\right)/\beta_n + \exp \left(-E_{a,2}/(R_T)\right) \) is the rate of heterogeneous reaction on the particles, \( \beta_n = \frac{\lambda_n(T) N_{t_D}}{c_g \rho_g r_p} \) is the particle mass transfer coefficient, \( N_{t_D} \) is the diffusion analogue of the Nusselt number.

The radii of particle were calculated by the formula:
\[
r_p = \left(\frac{3\rho_n}{4\pi \rho_g n_p} \right)^{1/3}.
\]

The friction force between particles and gas and the Nusselt number for calculating heat transfer between gas and particles are determined from the formulas [3].

3. Results and discussion
We have solved the problem (1–12) using the method based on the studies [5–6]. The detailed description of the used calculation algorithms is given in [3].

Parametric calculations have been performed for a suspension with the mass of the powder suspended in the air in the range from 0.03 kg/m\(^3\) to 0.05 kg/m\(^3\). The volume fraction of propane in the mixture varied from 1 to 2.5 percent. These values corresponded to an excess fuel ratio from 0.242 to 0.62. Particle radius varied from 0.5 to 2 \( \mu \)m. Other parameters were set according to table indicated values from the reference literature.

Figures 1–2 show the dependence of the apparent and normal combustion rate of a propane-air mixture and a coal-propane-air mixture with a mass fraction of particles of 0.05 kg/m\(^3\) on the propane
excess ratio in the mixture. It can be seen that the addition of coal dust significantly increases the combustion rate. The results presented in Figures 1 - 2 were obtained for mixtures with an excess of an oxidizing agent.

![Graph showing apparent combustion rate vs. excess fuel ratio](image1)

**Figure 1.** Dependence of the apparent combustion rate of the propane-air mixture and the coal-propane-air mixture on the excess fuel ratio. \( r_p = 1 \, \mu m \).

![Graph showing normal combustion rate vs. excess fuel ratio](image2)

**Figure 2.** Dependence of the normal combustion rate of a propane-air mixture and a coal-propane-air mixture on the excess fuel ratio. \( r_p = 1 \, \mu m \).

The results confirm the observations of authors from [6, 7]. In the presence of reactive particles, the velocity of flame propagation through the gas suspension increases.

On the other hand, in [8], the ambiguous influence of the presence of particles on the combustion rate of a gas suspension was shown. The modes of decreasing the flame propagation velocity during
the gas suspension in the presence of high concentrations of dust particles and with a low content of methane in the mixture are noted.

We performed calculations of the apparent combustion rate of a propane-air mixture of stoichiometric composition with the addition of coal dust particles (Figure 3). From the numerical solution of the problem it was obtained that for a stoichiometric mixture, coal dust particles reduce the apparent velocity of flame propagation. This is because the combustion reactions of gas and particles are competing. The more particles are in the mixture, the more oxidant is spent on their combustion. An interesting effect was also discovered with respect to the radius of the particles. An increase in the radius of the particles led to an increase in the apparent velocity of flame propagation. We attribute this to a decrease in the rate of consumption of the oxidizing agent by particles with an increase in their size.

![Figure 3. Dependence of the apparent combustion rate of a coal-propane-air mixture on the radii of the particles.](image)

**Conclusions**
A numerical study of the regularities of combustion of a coal-propane-air mixture has been carried out. The influence of the volumetric propane content, radius and mass concentration of particles on the visible and normal combustion rate of the mixture is shown. An ambiguous effect of the addition of coal dust particles on the combustion rate of the propane-air mixture has been obtained.

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