Mathematical model and calculation results of the kerosene aerosol combustion rate

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Abstract. This paper presents a mathematical combustion model of the kerosene aerosol and the calculation results of the combustion front normal velocity. The model is based on the dynamic equations of the two-phase reacting medium and consists of the energy equations for the gas and kerosene droplets, taking into account heat exchange, evaporation and heat release from the kerosene-oxygen reaction in the air; mass conservation equations for the gas, droplets, oxygen and kerosene, controlling the mass exchange between the phases and the burning of the reagents; the motion equation of the droplets; the particle number equations for the of droplets per unit volume; the ideal gas equation. The model assumes the isobaric conditions of the aerosol combustion. The obtained (calculated) propagation velocity of the kerosene aerosol combustion front, depending on the kerosene mass concentration and the initial temperature of the mixture, is in good agreement with the experimental data.

1. Introduction

Combustion of a liquid fuel aerosol is a very complex thermophysical and macrokinetic process. The beginning of combustion is preceded by evaporation of droplets and vapor mixing with the air. Since the kerosene vapor-air mixture is heated, a chemical reaction between the kerosene vapor and the oxygen in the air begins. The hot products of the reaction heat up unevaporated kerosene droplets, speeding up the process of their evaporation. All these processes occur directly in the reaction zone and in the warm-up zone prior to the reaction zone. The thickness of the vaporization zone depends on the temperature and the evaporation parameters of the fuel [1, 2]. To intensify the evaporation process of the droplets, nanoaluminum powder is added to kerosene [3]. The experimental study [3] has shown that a small amount of nanoaluminum powder in a kerosene drop (up to 1% by mass of the drop) leads to a 10% decrease in the evaporation time of the drop. Previously, we have numerically investigated the evaporation rate of a kerosene drop containing nanoaluminum particles [4]. The results of the numerical simulation coincide well with the experimental measurements of the kerosene droplet evaporation dynamics.

This study is devoted to the mathematical modeling of the kerosene aerosol combustion. The aim of the research is to develop a mathematical model of the combustion front propagation in the kerosene aerosol and conduct a calculation analysis of the influence of the kerosene mass concentration and the initial temperature of the aerosol on the combustion rate.
2. Problem statement
Kerosene aerosol is assumed to be uniformly distributed in a tube of large diameter and length with a closed end on the left and open one on the right. The tube has open end on the right and there is a high-temperature ignition spot (high temperature conditions), which ignites the aerosol. After the ignition at the right end, a combustion wave appears and starts propagating. The problem is to determine the dependence of the combustion wave propagation velocity on the mass concentration of kerosene droplets and the initial temperature of the aerosol.

As the aerosol is ignited and the combustion front starts spreading along the mixture, the gas expands and moves. It is supposed that the combustion of the aerosol proceeds under isobaric conditions. The droplets in the air prior to the combustion front start moving, heating up and evaporating. The evaporation of the droplets is described by the mass transfer coefficient. Since the temperature of the kerosene droplet reaches the boiling point, all the heat supplied to the drop is spent on evaporation. Kerosene vapors react with oxygen in the air. The reaction rate is defined by the second order Arrhenius law.

3. Mathematical combustion model
The mathematical model is based on models [4-6] and for the made assumptions consists of:

- gas continuity equation:
  \[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial x} = G_k, \]  

- oxygen mass balance equation:
  \[ \frac{\partial \rho_o}{\partial t} + \frac{\partial (\rho_o v)}{\partial x} = \frac{\partial}{\partial x} \left( \rho D \frac{\partial (\rho_o / \rho)}{\partial x} \right) - \frac{\alpha_o \rho_o}{\mu_k} \Phi(T), \]  

- kerosene vapor mass balance equation:
  \[ \frac{\partial \rho_f}{\partial t} + \frac{\partial (\rho_f v)}{\partial x} = \frac{\partial}{\partial x} \left( \rho D \frac{\partial (\rho_f / \rho)}{\partial x} \right) + G_k - \Phi(T), \]  

- kerosene droplets mass balance equation
  \[ \frac{\partial \rho_k}{\partial t} + \frac{\partial (\rho_k w_k)}{\partial x} = -G_k, \]  

- gas energy equation:
  \[ c \rho \left( \frac{\partial T}{\partial t} + v \frac{\partial T}{\partial x} \right) = \lambda \frac{\partial^2 T}{\partial x^2} + 4 \pi \alpha_k r_k^2 n_k (T_k - T) + G_k \left( c_k^e T_k - c T \right) + Q_k \Phi(T), \]  

- kerosene droplets energy equation:
  \[ c_k \rho_k \left( \frac{\partial T_k}{\partial t} + w_k \frac{\partial T_k}{\partial x} \right) = -4 \pi \alpha_k r_k^2 n_k (T_k - T) - L_k G_k, \text{ if } T_k < T_{up}, \]  

\[ T_k = T_{up}, \text{ if } T_k \geq T_{up}, \]  

- kerosene droplets motion equation
  \[ \frac{\partial w_k}{\partial t} + w_k \frac{\partial w_k}{\partial x} = -\tau_{w_k}, \]  

- number concentration equation for kerosene droplets:
\[
\frac{\partial n_k}{\partial t} + \frac{\partial (n_kw_k)}{\partial x} = 0,
\]

(8)

gas equation:
\[
p = \rho RT / \mu = \text{const}.
\]

(9)
The radius of the kerosene droplets is defined by:
\[
r_k = \left( \frac{\rho_k}{(4/3)\pi n_k \rho_k^5} \right)^{1/3}.
\]

(10)
The initial conditions:
\[
T(x,0) = \begin{cases} T_0, & 0 \leq x < x_b, \\ T_b, & x_b \leq x \leq l, \end{cases},
\]

\[
T_k(x,0) = T_b, \quad \rho(x,0) = \frac{\mu p}{RT(x,0)}, \quad \rho_o(x,0) = 0.2 \rho(x,0),
\]

\[
\rho_k(x,0) = \rho_{k,0}, \quad \rho_f(x,0) = \rho_{f,0}, \quad \nu(x,0) = 0, \quad w_k(x,0) = 0, \quad r_k(x,0) = r_{k,0}, \quad 0 \leq x \leq l.
\]

(11)
The boundary conditions:
\[
\frac{\partial T(0,t)}{\partial x} = 0, \quad \frac{\partial T(l,t)}{\partial x} = 0, \quad \frac{\partial T_k(0,t)}{\partial x} = 0, \quad \frac{\partial \rho(0,t)}{\partial x} = 0, \quad \frac{\partial \rho_o(0,t)}{\partial x} = 0, \quad \frac{\partial \rho_o(l,t)}{\partial x} = 0,
\]

\[
\frac{\partial \rho_f(0,t)}{\partial x} = 0, \quad \frac{\partial \rho_f(l,t)}{\partial x} = 0, \quad \frac{\partial \rho_k(0,t)}{\partial x} = 0, \quad \frac{\partial \rho_k(l,t)}{\partial x} = 0, \quad \nu(0,t) = 0, \quad w_k(0,t) = 0.
\]

(12)

Notations: \( t \) is the time; \( x \) is the coordinate along the tube; \( T \) is the gas temperature; \( T_k \) is the kerosene droplets temperature; \( T_o \) is the initial temperature of the aerosol; \( T_b \) is the temperature at the ignition area; \( \rho \) is the gas density; \( \rho_o \) is the partial density of oxygen; \( \rho_k \) is the distributed particle density; \( \rho_{k,0} \) is the liquid kerosene density; \( n \) is the number of the droplets per unit volume; \( \nu \) is the gas velocity; \( w_k \) is the droplets velocity; \( p \) is the pressure; \( r_k \) is the droplet radius; \( \mu, \mu_o, \mu_k \) are the molar masses of the air, oxygen and kerosene vapor; \( c \) is the air specific heat capacity at constant pressure; \( \lambda \) is the gas thermal conductivity coefficient; \( D \) is the diffusion coefficient; \( \alpha \) is the heat emission factor; \( G_k \) is the droplets mass change rate during combustion; \( Q_k \) is the kerosene combustion energy; \( R \) is the universal gas constant; \( r_f \) is the interaction force between the gas and droplets; \( l \) is the length of the aerosol cloud in the tube; and \( x_b \) is the left coordinate of the initial ignition spot (it has the length from \( x_b \) to \( l \)). \( G_k \) is the evaporation rate of kerosene droplets per unit volume determined as:
\[
G_k = -4\pi\alpha r_k^2 n_k \rho_k^0 \frac{dr_k}{dt}, \quad \frac{dr_k}{dt} = \begin{cases} \beta(\rho_f - \rho_{f,0})/\rho_k^0, & T_k < T_{\text{vap}}, \\ \frac{Nu \lambda}{r_k} (T_{\text{vap}} - T), & T_k = T_{\text{vap}}, \end{cases}
\]

\[
\rho_{f,0} = \frac{p_{f,0}}{R_k T_k}, \quad p_{f,0} = p \exp \left( \frac{L_k}{R_k T_k} + \frac{L_k}{R_k T_{\text{vap}}} \right).
\]

(13)
\[ Nu = 2 + \left( \frac{\text{Nu}_{l}^2 + \text{Nu}_{t}^2}{2} \right)^{1/2}, \quad \text{Nu}_{l} = 0.664 \text{Re}^{0.5}, \quad \text{Nu}_{t} = 0.037 \text{Re}^{0.8}, \quad \text{Re} = \frac{2r_k \rho |v - w_k|}{\eta}. \]

The heat emission factor is determined by the formula:

\[ \alpha_k = \frac{\text{Nu} \lambda}{2r_k}. \] (14)

To determine the mass transfer coefficient \( \beta \) the analogy of the processes of heat exchange and mass transfer have been used. The intensity of mass transfer is determined by the Sherwood number: \( Sh = \beta r_k (t)/D \), where \( D \) is the diffusion coefficient. Considering that the Lewis number for the gas \( Le = \frac{D}{\lambda / c P} = 1 \) and the equality \( Sh = \text{Nu} \), the mass transfer coefficient is defined as:

\[ \beta = \frac{D \cdot Sh}{r_k} = \frac{\lambda \text{Nu}}{c \rho r_k}. \] (15)

The interaction force between kerosene droplets and the gas is:

\[ \tau = \frac{F_{fr} - 4/3 \pi r_k^3 \rho_k^0}{c r_k}, \quad F_{fr} = C_{fr} S_m \rho (w_k - v) |v - w_k| \frac{r_k}{2}. \] (16)

The drag coefficient \( C_r \) is defined by the empirical formula from [7]:

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

where \( F_{fr} \) is the resistant force during the flow over the sphere; \( S_m \) is the middle section area; \( \eta \) is the absolute viscosity coefficient, and \( \text{Re} \) is the Reynolds number.

The chemical reaction rate between kerosene vapor and oxygen is described by the Arrhenius law:

\[ \Phi(T) = k_{0,K} \rho_{fr} \rho_O \exp\left(-\frac{E_{fr}}{(RT)}\right). \] (17)

\( E_{fr} \) is the reaction energy of activation, and \( k_{0,K} \) is the preexponential factor in the Arrhenius law.

### 4. Solution method and calculation results

The equation system of the mathematical model has been solved numerically by the method described in [5, 6]. A numerical study of the kerosene aerosol combustion has been carried out for the stoichiometric concentration of kerosene droplets and for lower values. The initial temperature of the aerosol has been varied in the range of \( T_0 = 293 \div 413 \text{ K} \), under the atmospheric pressure \( p = 0.1 \text{ MPa} \) and for the droplet size of \( r_{k,0} = 10 \mu m \).

The calculations have been performed at the following values of thermophysical and formal-kinetic quantities:

- \( c = 1000 \text{ J} / (\text{kg} \cdot \text{K}) \),
- \( R = 8.31 \text{ J} / (\text{mol} \cdot \text{K}) \),
- \( \eta = 2 \cdot 10^{-5} \text{ Pa} \cdot \text{s} \),
- \( \lambda = 0.1 \text{ W} / (\text{m} \cdot \text{K}) \),
- \( \rho_k^0 = 800 \text{ kg} / \text{m}^3 \),
- \( c_k = 2200 \text{ J} / (\text{kg} \cdot \text{K}) \),
- \( \mu_{o2} = 0.032 \text{ kg} / \text{mol} \),
- \( \mu = 0.029 \text{ kg} / \text{mol} \),
- \( \mu_k = 0.1 \text{ kg} / \text{mol} \),
- \( E_{fr} = 167.4 \text{ kJ} / \text{mol} \),
- \( k_{0,K} = 4 \cdot 10^{10} \text{ m}^3 / (\text{kg} \cdot \text{s}) \),
- \( T_{vap} = 175 \text{ °C} \),
- \( L_k = 222 \text{ kJ} / \text{kg} \),
- \( R_k = R / \mu_k \),
- \( Q_k = 40 \text{ MJ} / \text{kg} \).

The length of the tube \( l = 0.0156 \text{ m} \), and the length of the elevated temperature \( l - x_0 = 0.0031 \text{ m} \).

The combustion front propagation velocity has been determined as the motion speed of the oxygen partial density isoline equal to \( \rho_{fr} = 0.05 \text{ kg} / \text{m}^3 \).
First, we have matched the calculation results with the experimental data on the combustion rate of the kerosene aerosol. Experimental data on the dependence of the combustion rate on the initial temperature under the stoichiometric ratio of the air and kerosene and on the mass concentration of kerosene in the air at the initial temperature of 20°C are presented in [1]. The matching of the calculation results with the experimental data has been carried out by defining the value of \( k_{0,K} \), at which the flame propagation velocity coincides with the experimental value under the stoichiometric ratio of the air and kerosene at 40°C. The calculations have been conducted using the model (3) - (15). The aim of the calculations was to determine the combustion front propagation velocity depending on the initial temperature of the aerosol under the stoichiometric ratio of the air and kerosene and depending on the mass concentration of kerosene at the initial temperature of 20°C. The example of one calculation is presented in figure 1.

\[ l = 0.0156 \, m, \quad l - x_0 = 0.0031 \, m, \quad \rho_{k,0} = 0.05 \, kg/m^3, \quad T_0 = 293 \, K, \quad r_{k,0} = 10 \, \mu m. \]

Figure 1 illustrates the stages of establishing the stationary propagation mode of the combustion front. The temperature of the gas and droplets increases in the combustion front (figure 1 a, b), kerosene droplets evaporate (d), the air density decreases (e) and the oxygen partial density becomes lower. The kerosene partial density grows due to the droplet evaporation and then decreases because of the chemical reaction. The gas velocity behind the combustion front grows up to 1.35 m/s due to the thermal expansion of the gas under the constant pressure conditions. The speed of the combustion front propagation reaches 0.23 m/s.

Figures 2 and 3 show the dependences of the combustion front propagation velocity in the aerosol on the initial temperature of the kerosene aerosol and on the kerosene mass concentration of in the
mixture. As it can be seen from the figures, there is a good agreement of the calculation results by model (1)-(17) with experimental data.

![Graph 1](image1)

![Graph 2](image2)

**Figure 2.** The dependence of the combustion front propagation velocity on the initial temperature of the kerosene aerosol. The equivalence ratio is 0.95. (calculation results-dotted line, experimental data from [1]-solid line)

**Figure 3.** The dependence of the combustion front propagation velocity on the kerosene mass concentration (calculation results-dotted line, experimental data from [1]-solid line)

5. Conclusion
This paper has presented a mathematical combustion model of kerosene aerosol in the air. The developed model can be applied for numerical simulation of combustion of different flammable liquids sprayed in the air. The conducted numerical study using the developed model allowed obtaining the dependence of the flame propagation velocity in the kerosene aerosol on its initial temperature and on the mass concentration of kerosene droplets. The obtained results are in good agreement with experimental data.

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