Numerical investigation on burning rate of propane-air mixture

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Abstract. The paper presents a physico-mathematical model and calculation of the burning rate of a propane-air mixture. The problem formulation includes the equations of mass, momentum and energy conservation for the gas, supplemented by the equations of the oxidizer and fuel mass conservation in the gas. Godunov’s scheme is used to solve the equation system of the model. The paper provides the result of the numerical simulation on the apparent and normal burning rates of the propane-air mixture. The obtained calculation results are in reasonably good agreement with the known studies of other authors.

1. Introduction
To design efficient burner devices capable of operating in extreme conditions, it is necessary to accurately predict the burning rate of the fuel. In our previous study [1] we have calculated the burning rate of a methane–air mixture. The calculation result accurately coincided with the data from [2] and [3]. According to the study [3], methane-air mixture begins to burn at a methane volume fraction of about 5.2% [3]. While as the propane-air mixture ignites at lower volume concentrations. Therefore, in some cases it is more convenient to use a propane-air mixture as a fuel.

The aim of this study is to develop a physico-mathematical model of a propane-air mixture combustion and conduct a numerical study on the dependence of the normal and apparent burning rate of the mixture on the excess fuel coefficient.

2. Mathematical model
The mathematical model is formulated under the following assumptions: there is a volume filled by a reactive mixture with a volume concentration of the combustible component \( \alpha_f \). The mixture is capable of exothermic chemical reaction when heated. Radiant heat transfer of the combustion products is neglected. The molecular dissociation of the combustion products at high temperature is assumed to be absent. The diffusion and thermal conductivity coefficients are temperature dependent. The gas constant is determined by the composition of the gas mixture. The rate of the chemical reaction depends on temperature according to the Arrhenius law, the reaction rate depends on the concentration of propane and oxygen, and is described by first-order kinetics for propane and first-order for oxygen. The gas motion due to the thermal expansion with increasing temperature is taken into account. Under the made assumptions the problem formulation has the form:

the continuity equation:

\[
\frac{\partial \rho_f}{\partial t} + \frac{\partial \rho_f u_f}{\partial x} = 0,
\]
the impulse-conservation equation:
\[
\frac{\partial (\rho_g u_g)}{\partial t} + \frac{\partial (\rho_g u_g^2 + p_g)}{\partial x} = 0,
\]
(2)
the energy equation:
\[
\frac{\partial \rho_g \left( e_g + 0.5u_g^2 \right)}{\partial t} + \frac{\partial \left[ \rho_g \left( e_g + 0.5u_g^2 \right) + p_g \right] u_g}{\partial x} = \frac{\partial}{\partial x} \left( \lambda_g \frac{\partial T_g}{\partial x} \right) + Q_{ch} W_{ch},
\]
(3)
the mass balance equation of the combustible component in the gas:
\[
\frac{\partial \rho_{\text{ch}}}{\partial t} + \frac{\partial \rho_{\text{ch}} u_g}{\partial x} = \frac{\partial}{\partial x} \left( D_{ch} \rho_{ch} \frac{\partial \rho_{\text{ch}}}{\partial x} \right) - W_{ch},
\]
(4)
the oxygen mass balance equation in the gas:
\[
\frac{\partial \rho_{\text{ox}}}{\partial t} + \frac{\partial \rho_{\text{ox}} u_g}{\partial x} = \frac{\partial}{\partial x} \left( D_{ox} \rho_{ox} \frac{\partial \rho_{\text{ox}}}{\partial x} \right) - \alpha_W W_{ch},
\]
(5)
the perfect-gas law:
\[
\rho g = \rho_f \gamma \rho_{ch} T_g,
\]
(6)
the initial conditions:
\[
T_g (x,0) = \begin{cases} T_{b}, & 0 \leq x \leq x_0 \\ T_{gb}, & x_0 < x \leq \infty \end{cases},\quad \rho_f (x,0) = \rho_{f,b}, \quad \rho_{\text{ch}} (x,0) = \rho_{\text{ch},b}, \quad \rho_{\text{ox}} (x,0) = 0, \quad p_g (x,0) = p_{gb},
\]
(7)
the boundary conditions:
\[
\frac{\partial \rho_g (0,t)}{\partial x} = \frac{\partial \rho_g (x,t)}{\partial x} = \frac{\partial \rho_{\text{ch}} (0,t)}{\partial x} = \frac{\partial \rho_{\text{ch}} (x,t)}{\partial x} = \frac{\partial \rho_{\text{ox}} (0,t)}{\partial x} = \frac{\partial \rho_{\text{ox}} (x,t)}{\partial x} = 0,
\]
(8)
(9)
Notations: \( \rho_f \) and \( \rho_{\text{ox}} \) are the partial densities of fuel and oxygen in the mixture \( \rho_f = a_f \rho_{ch} \), \( \rho_{\text{ox}} = a_{\text{ox}} \rho_{ch} \), where \( a_f, a_{\text{ox}} \) are the mass concentrations of the combustible component and oxygen in the gas; \( e_g = \gamma \rho_f \gamma \rho_{ch} \) is the gas energy; \( \gamma = \gamma_f / \gamma_g \) is the adiabatic exponent; \( \rho \) is the density, \( u \) is the velocity, \( t \) is the time, \( x \) is the coordinate; \( p \) is the pressure, \( T \) is the temperature; \( Q_{ch} \) is the thermal effect of the reaction; \( k_0 \) is the rate constant of the chemical reaction; \( \alpha_W = \mu_{\text{ox}} \gamma_{\text{ox}} / \mu_f \gamma_f \) is the oxygen consumption coefficient in the reaction with propane; \( \mu_{\text{ox}}, \mu_f \) are the molar masses of oxygen and propane; \( \gamma_{\text{ox}}, \gamma_f \) are the stoichiometric reaction coefficients; Subscript: \( b \) is for the initial values of the state parameters, \( g \) - gas parameters, \( \text{ox} \) - oxygen, \( f \) - propane. The chemical rate is determined by the right-hand sides of equations (3) – (5):
\[
W_{ch} = \rho_f \rho_{\text{ox}} k_0 \exp \left( -E_r / (R_g T_g) \right).
\]
The connection between the mass concentration of the combustible component and the oxidizer in the gas with the volumetric content of the combustible component \( a_{\text{vol}} \) in the mixture is defined from the ratios:
The results do not exactly repeat the assumptions of the mathematical model and the error of the experimental data [3].

The normal burning rate corresponding to the partial density of the combustible component 10 times greater than 0.52%.

The difference between the apparent burning rate and the gas velocity.

The diffusion and thermal conductivity coefficients of the gas depend on temperature as in [1]:

\[
\lambda_g = \lambda_0 \left( \frac{T_g}{T_0} \right)^{2/3}, \quad D_g = \lambda_g \left( c_s \rho_g \right),
\]

where \( \lambda_0 \) is the value of the thermal conductivity at \( T_g = 300K \).

The gas constant depends on the composition of the mixture and is defined as

\[
R_g = R_g \left( a_{\text{m}} \mu_{\text{m}} + a_j \mu_j + (1 - a_{\text{m}} - a_j) \mu_{N2} \right),
\]

where \( \mu_{N2}, \mu_{\text{m}} \) are the molar masses of nitrogen and oxidizer.

The problem (1) – (6) with boundary and initial conditions (7) – (9) is solved numerically using Godunov’s scheme [4]. The spatial step is equal to \( \Delta h_g = 10^{-5} \text{ m} \). The size of the computational domain is chosen so that during the ignition and the combustion wave formation, the shock wave arising from the energy release in the ignition zone does not reach the boundary of the domain. The time step is determined by Courant–Friedrichs–Lewy condition as

\[
\Delta t = \min \left[ \frac{0.2 \Delta h_{\text{min}}}{\max [c] + \max [\mu_g]}, \frac{\Delta h_{\text{min}}^2}{\chi_g} \right],
\]

where \( c \) is the sound speed, \( \chi_g \) is the temperature conductivity of the gas. The algorithm of the numerical solution and the program code has been verified similarly to [1]. The error of the calculation is no more than 0.52%.

### 3. Results and discussion

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

- \( Q_{1b} = 42.45 \text{ MJ/kg}, \ E_a = 171.16 \text{ kJ/mol}, \ R_a = 8.311 \text{ J/(mol·K)}, \ x_0 = 2 \cdot 10^{-3} \text{ m}, \ T_0 = 1500 \text{ K}, \ T_g = 300 \text{ K}, \end{equation}
- \( \lambda_0 = 0.025 \text{ W/(m·K)}, \ \mu_g = \left( \rho_g a_{\text{air}} + \rho_j a_{f,b} \right) / \left( \rho_{\text{air}} a_{\text{air}} + \rho_j a_{f,b} / \mu_j \right), \ R_g = 8.31 \mu_g / \left( \text{kg · K} \right), \end{equation}
- \( a_1 = 3.64, \ c_{pg} = 29.174 \mu_g^{-1} / \left( \text{kg · K} \right), \ c_{vg} = 20.864 \mu_g^{-1} / \left( \text{kg · K} \right), \ \mu_{\text{air}} = 29.04 \cdot 10^{-3} \text{ kg / mol}, \end{equation}
- \( \mu_j = 44 \cdot 10^{-3} \text{ kg / mol}, \ \rho_j = 1.83 \text{ kg / m}^3, \ \rho_{\text{air}} = 1.2 \text{ kg / m}^3, \end{equation}
- \( p_{gb} = 0.1 \text{ MPa}. \end{equation}

We have conducted the test numerical simulation to determine the preexponential factor \( k_0 \). We have tuned the factor \( k_0 \) to simulate the normal combustion rate of the propane-air mixture with the fuel excess coefficient \( \phi = 0.85 \) according to the study [3]. The tuned value of the coefficient \( k_0 \) is equal to \( 5 \cdot 10^{10} \text{ m}^3/(\text{kg·s}) \). In further calculations, the value of the fuel excess coefficient varies in the range of \( \phi = 0.5 \pm 1 \). The aim of the calculations is to define the normal and apparent burning rate of the propane-air mixture. The apparent burning rate of the propane-air mixture is defined as the velocity of the coordinate corresponding to the partial density of the combustible component 10 times lower than the initial value. The normal burning rate is equal to the difference between the apparent burning rate and the gas velocity. The calculation results are shown in Figures 1, 2.

Figure 1 shows the comparison of the calculated results with the data from [3]. As it can be seen from the figure, the results do not exactly repeat the data from [3]. The reason may be both the assumptions of the mathematical model and the error of the experimental data [3].
Figure 1. The normal burning rate depending on the fuel excess coefficient.

Figure 2. The apparent burning rate depending on the fuel excess coefficient.

Figure 2 shows the calculation results of the apparent flame propagation speed in the propane-air mixture. The lower flammability limit agrees with the data from [3]. For the propane-air mixture, the lower flammability limit is at the fuel excess coefficient $\phi = 0.5$, which corresponds to the 2% propane volume fraction in the mixture. According to Figure 2, the apparent burning rate of the propane-air mixture is close to zero as the fuel excess coefficient tends to the lower flammability limit.

4. Conclusions
We have developed the mathematical model of the propane-air mixture combustion. The paper provides the dependences of the visible and normal combustion front propagation velocity in the propane-air mixture on the coefficient of excess fuel in the gas. Numerical investigation has shown that for the mixtures with propane content close to the lower flammability limit, the normal and visible burning rate tends to zero. The burning rate of the poor propane-air mixtures is an order of magnitude less than the normal and visible burning rate of a stoichiometric mixture. The obtained calculation results are in reasonably good agreement with the known studies of other authors.

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