

NUMERICAL SIMULATIONS OF LEAN PROPANE-AIR FLAMES PROPAGATING IN CIRCULAR TUBES UNDER QUENCHING CONDITIONS

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Abstract

Flame extinction in internal combustion engines can be observed when a flame front enters a small gap between the cylinder and piston or above the piston rings. This phenomenon is caused by the interaction of the flame with the walls. Cooling of the reaction zone by the wall is the reason for the flame extinction. Simplifying the problem to the propagation of a premixed laminar flame in the narrow channels with isothermal wall allowed employing numerical methods to analyze this phenomenon. The aim of this work was to examine flame behavior during its propagation in the narrow circular tube. A numerical analysis of the freely propagating flame was conducted. In this study, the propagation and quenching of a laminar premixed propane/air flame in circular tube was investigated numerically. The flame chemistry is modeled by one-step overall reaction. The considerations are limited to flames propagating downwards in lean propane-air mixtures. Quenching diameter as a function of equivalence ratio was determined. One of the most important flame parameters - flame propagation velocity (under quenching conditions) was compared with adiabatic burning velocity and limit burning velocity predicted by Zeldovich. It was found satisfactory agreement between numerical calculations and theoretical considerations. Numerical results show also that there is a close dependence between preheat zone and dead space for flames propagating in a wider tube.

Keywords: flame quenching, flame propagation velocity, simulation

1. Introduction

Flame-wall interaction is important for understanding the combustion process near a wall. Every flame can be quenched in a narrow channel, if the distance between the walls is small enough. Heat loss from the flame to the walls is responsible for flame quenching. The first extensive survey and analysis of quenching distance problems was made by Potter [1]. According to his analysis, the quenching distance depends on fuel type, mixture concentration and direction of flame propagation. Later, the quenching distance and flame properties accompanying quenching conditions were studied for flames propagating in methane/air mixtures (Jarosinski, [2]) and later in propane/air mixtures (Jarosinski and Podfilipski, [3]). For flames in lean methane/air and rich propane/air mixtures ($Le < 1$) the quenching distance depends on the direction of flame propagation, upward or downward. Flame stretch and preferential diffusion are the physical factors responsible for the difference between the two directions of propagation.

Theoretical and numerical analysis of the properties of a flat flame during its propagation near a cold wall was made by von Kármán and Millan [4]. Two-dimensional simulations of quenching and flame shape were presented by Aly and Hermance [5]. They calculated isotherms for a near quench flame propagating in a parallel plate channel. Later Lee and T'ien [6] and Lee and Tsai [7] presented numerical study of flame quench and flame structure in circular tubes. They consider both isothermal and adiabatic walls. They also identified two basic classes of flame structure, which propagate in tubes. First structure, the tulip shaped flame, is concave in the direction of propagation at the centerline. The other, mushroom shaped flame, is convex at the centerline in the propagation direction.

Recently, numerical investigation of unsteady premixed flames in narrow channels with adiabatic and isothermal walls was presented in a paper of Song et al. [8]. They confirmed the existence of mushroom and tulip shaped flames depending on boundary conditions and the ignition method. Also, Maruta and et al. [9] investigated experimentally, analytically and numerically, the characteristics of combustion in a channel with an inner diameter smaller than the conventional quenching distance, which was possible with heated channels wall.

The aim of this work was to examine flame behavior during its propagation in the narrow circular tube. A numerical analysis of the freely propagating flame was conducted.

2. Numerical Model

A combustion process of premixed propane/air mixture in cylindrical tube is considered. A mathematical model capable of predicting the reacting compressible flows was formulated based on the following assumptions: the system is axisymmetrical and radiation and Soret and Dufour effects are ignored. A schematic of the system is shown in Fig. 1.

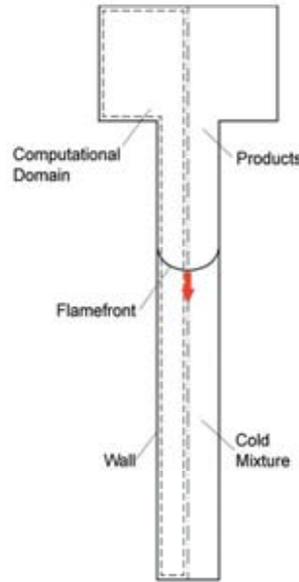


Fig. 1. Schematic of the computational domain (not to scale for ease of visualization)

The governing equations describing the gaseous flow are written in a cylindrical coordinate system (x, r) , where x-axis is chosen lie along the centerline of the tube. The velocity components u and v are in x and r directions, respectively. The governing equations can be written as follows:

Continuity equation:

$$\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x} (\rho u) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v) + \frac{\rho v}{r} = 0. \quad (1)$$

Momentum equations:

$$\begin{aligned} \frac{\partial}{\partial t} (\rho u) + \frac{1}{r} \frac{\partial}{\partial x} (r \rho u u) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho v u) = \\ - \frac{\partial p}{\partial x} + \frac{1}{r} \frac{\partial}{\partial x} \left[r \mu \left(2 \frac{\partial v}{\partial x} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right) \right] + \rho g, \end{aligned} \quad (2)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho v) + \frac{1}{r} \frac{\partial}{\partial x}(r \rho u v) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v v) = \\ - \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial x} \left[r \mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial r} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(2 \frac{\partial v}{\partial r} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] - 2 \mu \frac{v}{r^2} + \frac{2}{3} \frac{\mu}{r} (\nabla \cdot \vec{v}) + \rho \frac{v^2}{r}. \end{aligned} \quad (3)$$

Energy equation:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x}(\rho u h) + \frac{1}{r} \frac{\partial}{\partial r}(\rho v h) = \\ \frac{\partial}{\partial x} \left[k \frac{\partial T}{\partial x} + \sum_i \left(\rho D_i h_i \frac{\partial Y_i}{\partial x} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(k \frac{\partial T}{\partial r} + \sum_i \left(\rho D_i h_i \frac{\partial Y_i}{\partial r} \right) \right) \right] - r \sum_i^5 h_i \omega_i M_i. \\ (\omega_i = \gamma_i \omega_{C_3H_8} \quad i=1,2,\dots,5), \end{aligned} \quad (4)$$

Species equations:

$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x}(\rho u Y_i) + \frac{1}{r} \frac{\partial}{\partial r}(\rho v Y_i) = \frac{\partial}{\partial x} \left(\rho D_i \frac{\partial Y_i}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \rho D_i \frac{\partial Y_i}{\partial r} \right) + r \omega_i M_i. \quad (5)$$

Equation of state:

$$p = \rho R_u T \sum_i \frac{Y_i}{M_i}, \quad (6)$$

where

$$\nabla \cdot \vec{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial r} + \frac{v}{r}, \quad (7)$$

where:

P - denotes density,

p - pressure,

g - the gravitational acceleration,

T - temperature,

R_u - universal gas constant,

h - specific enthalpy ($h = \sum_i Y_i h_i$),

γ_i - stoichiometric ratio, ω_i the mass generation rate per unit volume,

Y_i - the mass fraction of species,

M_i - is the molecular weight of species.

The fluid viscosity μ , specific heat $c_{p,f}$, and thermal conductivity k are calculated from a mass fraction weighted average of species properties:

$$\mu = \sum_i Y_i \mu_i, \quad c_{p,f} = \sum_i Y_i c_{p,i}, \quad k = \sum_i Y_i k_i. \quad (8)$$

The species specific heat is calculated using piecewise polynomial fit of temperature. To evaluate local mass diffusivity coefficients for each species in the flame, the classic kinetic theory for low-density gases was employed. It was also used for evaluating thermal conductivity and molecular viscosity in the mixture:

$$D_{ij} = 0.0188 \frac{\left[T^3 \left(\frac{1}{M_i} + \frac{1}{M_j} \right) \right]^{1/2}}{p \sigma_{ij}^2 \Omega_D}, \quad (9)$$

$$k_i = \frac{15}{4} \frac{R}{M_i} \mu_i \left[\frac{4}{15} \frac{c_{p,i} M_i}{R} + \frac{1}{3} \right], \quad (10)$$

$$\mu_i = 2.67 \times 10^{-6} \frac{\sqrt{M_i T}}{\sigma^2 \Omega_\mu}, \quad (11)$$

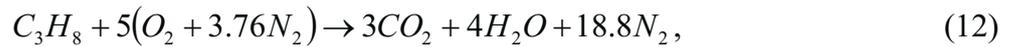
where:

Ω_D - is the diffusion collision integral,

σ - particle diameter,

Ω_μ - reduced collision integral.

A reduced one-step propane/air reaction model and fuel consumption rate $\omega_{C_3H_8}$ are given by equations (12) and (13) respectively:



$$\omega_{C_3H_8} = A \exp\left(-\frac{E_k}{RT}\right) [C_3H_8]^a [O_2]^b, \quad (13)$$

where the activation energy E_k is 1.256×10^8 J/kgmol, the preexponential factor A is 4.836×10^9 and parameters a and b are 0.1 and 1.65, respectively, as recommended by Westbrook and Dryer [10].

Numerical simulations were carried out for 3 mm channel with isothermal wall conditions ($T_{wall} = 288.15$ K). Ignition is located in wider tube (20 mm length), which later evolves into narrow channel.

3. Results and Discussion

Two cases were considered. The first one, where flame propagating in a certain mixture concentration close to quenching limit is able to exist after entering a narrow tube, and the second one, where flame propagating in a little leaner mixture is going to be quenched, while entering a narrow tube. These two mixture concentrations were found to be equal to $\Phi = 0.800$ and $\Phi = 0.795$, respectively. For the case of flame propagation, profiles of temperature and reaction rate are shown in Fig. 2a. Mass fractions of five species are shown in Fig. 2b.

Fig. 3a shows a comparison of the two cases in terms of flame positions versus time. There is no big difference until the narrow tube entrance (dashed line) is reached by flames. After crossing the narrow tube edges the lines refract and progressively split each other. The flame propagation line is going to be linear, whereas the flame quenching line loses its linearity and stops, what correspond to flame extinction. These lines were used to calculate flame propagation velocities, which are shown in Fig. 3b. At the top end of a wider diameter tube the energy was supplied to ignite the mixture as a result of that high values of flame velocities are visible. These values are fixed in a short time and finally are equal to 28.42 cm/s for propagation and to 26.87 cm/s for quenching. Interesting flame behavior is observed in front of the narrow tube entrance. When flame approaches it propagation velocity increases. These velocities reach the maximum values about 38 cm/s and 36.7 cm/s and later sharply decrease. For the quenching case flame propagation

velocity decreases to zero, whereas for flame propagation its value is settled at a level of $S_{L,q} = 15.24$ cm/s, what is about 54% of the value in the wider tube. It is surprising that a flame propagation velocity increases close to the entrance of a narrow tube. It is the result of interaction of flame with a narrow tube entrance, resulting in increase of flame area. Flame shape evolution can be observed in Fig. 4. The numbers correspond to characteristic points indicated in Fig. 3b.

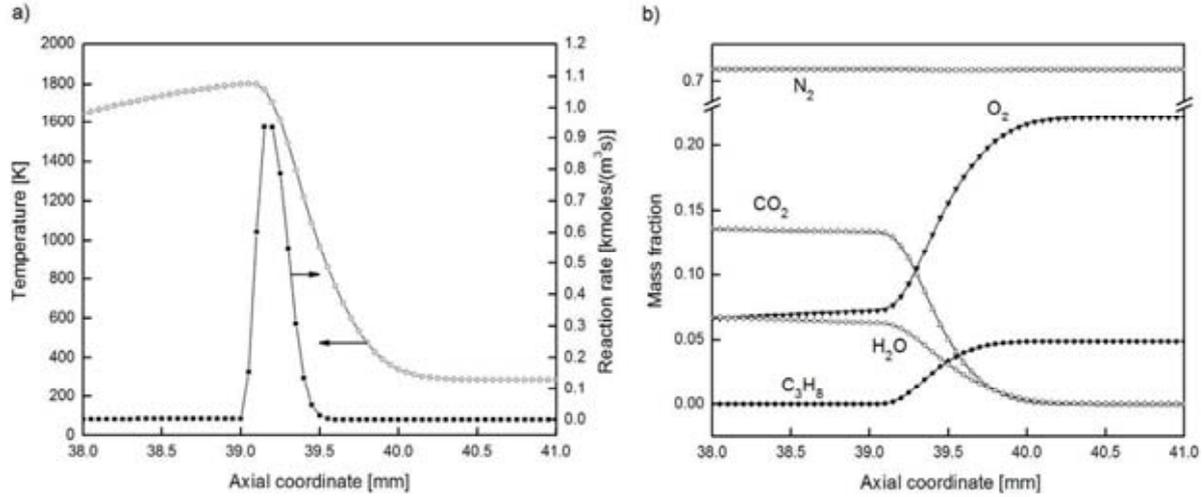


Fig. 2. Structure of flame propagating in channel 3mm and in mixture with equivalence ratio $\Phi = 0.800$: (a) variation of temperature and reaction rate, (b) distributions of the mass fraction of the five species

The problem of flame quenching by walls was theoretically explored by Zeldovich [11, 12]. He found a relation between laminar burning velocity at the quenching limit $S_{L,lim}$ and adiabatic laminar burning velocity S_L :

$$\frac{S_{L,lim}}{S_L} = e^{-\frac{1}{2}} = 0.61. \quad (14)$$

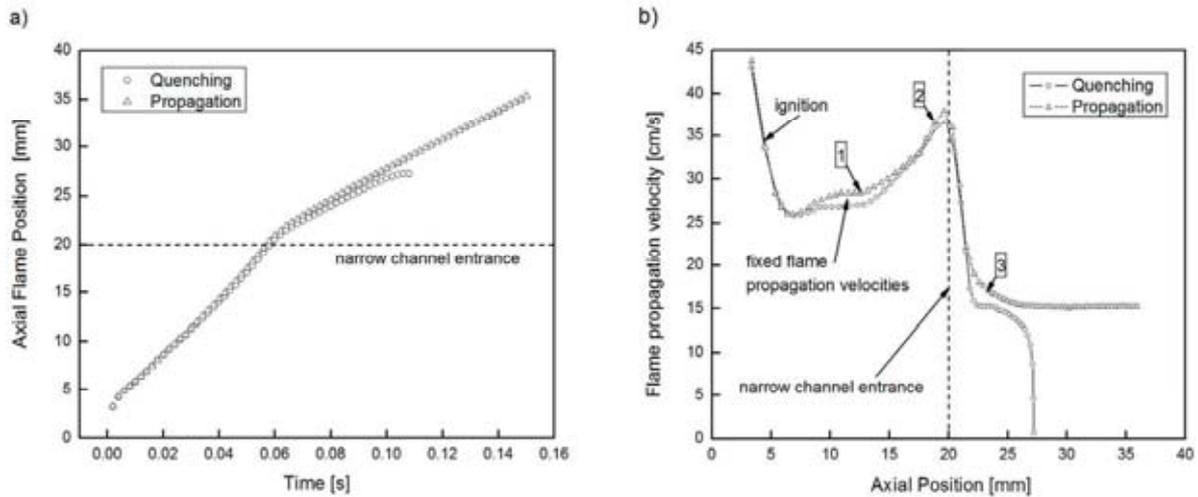


Fig. 3. Flame positions as a function of time (a) and flame propagation velocity as a function of flame position (b) for flame propagation ($\Phi = 0.800$) and flame quenching ($\Phi = 0.795$)

To compare flame propagation velocity obtained from numerical simulations for laminar burning velocity at the quenching limit it is necessary to know adiabatic laminar burning velocity for $\Phi = 0.800$. This value can be found in the paper of Vagelopoulos and Egolfopoulos [13] and it

is equal to 30 cm/s. It follows from Eq. 14 that $S_{L,lim} = 18.3$ cm/s. The difference between a calculated value of $S_{L,q}$ and the theoretical prediction of Zeldovich $S_{L,lim}$ is relatively small.

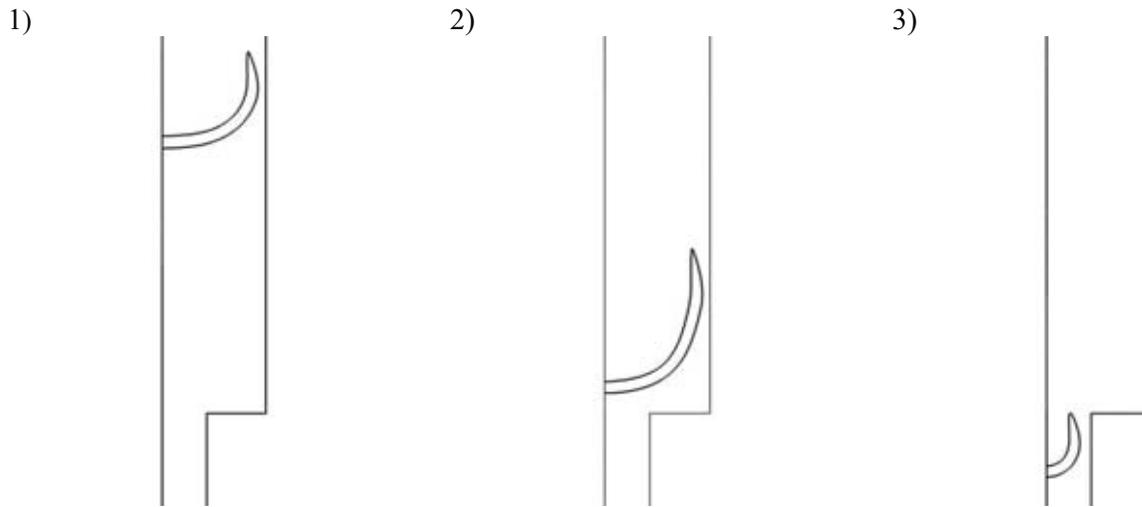


Fig. 4. Flame shape evolution during its propagation from the wide to narrow tube for $\Phi = 0.800$. Numbers correspond to positions in Fig. 3

Another important parameter for flame propagating close to quenching conditions is dead space. Here, it is defined as the minimum distance from the wall to the peak of the reaction rate in the radial direction. Analyzing the case of flame propagation it can be noticed that dead space increases from 0.25 mm for wider channel to 0.32 mm for narrow channel. It means that for sufficiently large tube, dead space is similar to the preheat zone of the adiabatic flat flame, which is equal in this case to 0.19 mm.

4. Conclusions

In this study, the propagation and quenching of a laminar premixed propane/air flame in circular tube was investigated numerically. Simulations show that flame propagation velocity at the entrance to the narrow tube increased due to the increase of the flame area. Flame propagation velocity in a narrow tube is equal to 15.24 cm/s what is close to the theoretical predictions. Dead space under quenching conditions is larger than for the flame propagating under condition, where heat losses do not play important role.

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