INFLUENCE OF NUMBER OF STEP REACTIONS ON FLAME PARAMETERS UNDER QUENCHING CONDITIONS

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Abstract

Last decade, construction and using of microscale gas-turbines and internal combustion engines is collecting growing attention. However, the flame propagation limitations impede the development of micro and mesoscale combustion devices. Due to its small scale, increasing effect of flame–wall interaction causes a large heat loss and in consequence flame quenching. Both, fundamental experimental work and numerical simulations are conducted in order to overcome quenching issues. The most basic analysis concerns flame behaviour in small scale devices are premixed flame propagation in narrow tubes. There are two possibilities of flame-flow configurations: flame moving in a stationary mixture and a stationary flame in mowing mixture. These configurations have influence on flame shape, flame propagation velocity and quenching diameter. Most of numerical investigation assumes single-step reaction. It means that for flames propagating in propane-air mixtures C_3H_8 reacts directly with oxygen and leads to CO_2 and H_2O. This chemical kinetics mechanism omits existence of CO in reaction zone and in combustion products. Therefore it is interesting to use two-step reactions mechanism and compare the results with those obtained from single-step reaction model. The purpose of this analysis is to find influence of number of reaction steps on flame behaviour under quenching conditions for flames propagating in stationary lean propane-air mixtures. Quenching diameter, flame propagation velocity are determined and analyzed.

Keywords: *flame propagation, quenching diameter, flame propagation velocity, numerical simulation*

1. Introduction

Micro-scale power systems, where combustion of hydrocarbon fuels is used, are considered as the alternatives to lithium-ion batteries due to their higher energy density per unit mass or unit volume. However, constructing small-scale combustors is charging some difficulties. They arose due to using low Reynolds numbers in these devices, so turbulent mixing cannot be sustained in order to accelerate the burning rate. Another problem is that thermal losses increase dramatically as the size of the device is reduced. The smaller tube diameter (or distance between walls) in which flame is able to propagate for certain mixture concentration is call a quenching diameter (or quenching distance). Decreasing it will lead to flame extinguish, it has been shown experimentally that combustion can be maintained in channel smaller than the quenching diameter but it requires a wall temperature high enough [1]. Many experimental works has been conducted for understanding the flame propagation characteristic in small-scale channels [2, 3]. The former study concerned flame stabilization in tubes of different diameters, while the latter analyzed flame propagation in a cylindrical tube with a wall temperature along the direction of fluid flow. Numerical simulations of flames propagating in narrow channels have been developed parallel with an experimental investigation. The most important works, which should be mentioned here were prepared by: Aly and Hermance [4], Lee and Tsai [5], Hackert et al. [6] and Kim and Maruta [7]. They have analyzed various configurations of flames propagating in stationary or moving stoichiometric mixtures, with different thermal conditions of the wall (adiabatic or isothermal).

Development of computation fluid dynamic (CFD) tools, allows using them to design small-scale combustors. Therefore it is important to compare results obtained from one of the most

popular CFD code - ANSYS-Fluent [8] for typical configuration of flame propagation in narrow tubes with experimental data. This paper addresses the influence of number of step reactions on the flame behaviour close to quenching limit for several tube diameters. One and two-step reaction mechanism model were used to obtain mixtures concentrations and flame propagation velocity under quenching conditions and compared them with experimental results.

2. Computational details

The details of the computational domain used for the present numerical studies are presented in Fig. 1. Every computational domain consists of two cylinders: wider and narrower. The diameters of narrower tubes are 3 mm, 5 mm, 7 mm and 9 mm. Computations were solved numerically using the CFD on a block structured grid, with the finest grid covering the flame zone and following it all the time. The work of Kim and Maruta [7] demonstrated how the dimensions of the grid affect the error associated with computing the flame propagation velocity. This is the reason why in the vicinity of the flame the grid dimensions do not exceed 50 μm × 50 μm which should ensure an error in determination of flame propagation velocity on the level of 0.5%.

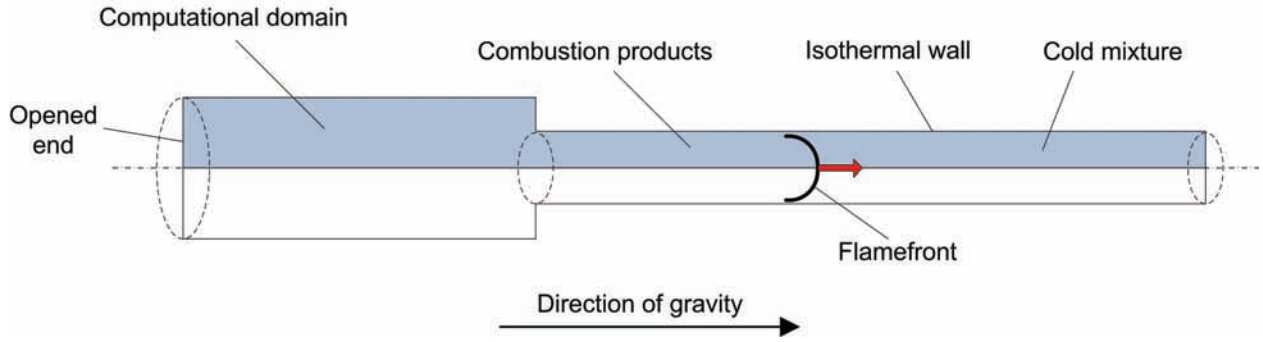

Fig. 1. Schematic of the computational domain (not to scale for ease of visualization)

In the present studies, 2-D laminar premixed flame propagation in propane/air mixtures in half of the tubes is considered due to the axysimmetrical shape along the central axis. The thermodynamics properties of fuel/air mixtures and combustion product as well are assumed to depend on temperature. The density of the fluid is calculated using ideal gas law. The specific heat, thermal conductivity and viscosity of the mixtures are calculated using a mass weighted average of species properties. These properties for the individual species are determined from piecewise polynomials (for specific heat) and from kinetic theory for low-density gases (for thermal conductivity and viscosity). Kinetic theory relations are also used to evaluate the local mass diffusivity of the mixture. A set of equations corresponding to full Navier-Stokes model for reactive flows was used. For the sake of simplicity, the following assumptions are used:

- the swirl velocity component is 0,
- no Soret and Dufour effects,
- no gas radiation,
- no work done by pressure and viscous forces,
- reaction mechanisms involving multi-species and one and two-step reactions.

The governing equations describing the gaseous flow are written in a cylindrical coordinate system (x, r), where x-axis is chosen along the centreline of the tube. The velocity components u and υ are in x and r directions, respectively. With the above assumptions, the governing equations for the transient premixed flame can be written as follows:

For the overall mass balance we have

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{1}{r}\frac{\partial (\rho \upsilon r)}{\partial r} = 0, \tag{1}$$

where ρ is the density.

The x momentum is

$$\frac{\partial(\rho u)}{\partial t}+\frac{\partial(\rho uu)}{\partial x}+\frac{1}{r}\frac{\partial(\rho \upsilon u r)}{\partial r}=-\frac{\partial p}{\partial x}+\frac{\partial}{\partial x}\left(\frac{4}{3}\mu\frac{\partial u}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu\frac{\partial u}{\partial r}\right)$$
$$-\frac{\partial}{\partial x}\left(\frac{2\mu}{3r}\frac{\partial(\upsilon r)}{\partial r}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu\frac{\partial \upsilon}{\partial x}\right)+r\rho g\,, \tag{2}$$

where μ is the viscosity, g is gravitational acceleration, and p is the pressure.

The r momentum is

$$\frac{\partial(\rho \upsilon)}{\partial t}+\frac{\partial(\rho u \upsilon)}{\partial x}+\frac{1}{r}\frac{\partial(\rho \upsilon \upsilon r)}{\partial r}=-\frac{\partial p}{\partial r}+\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial r}\right)-\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{2r\mu}{3}\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial x}\left(\mu\frac{\partial \upsilon}{\partial x}\right)$$
$$+\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{4r\mu}{3}\frac{\partial \upsilon}{\partial r}\right)-\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{2}{3}\mu\upsilon\right). \tag{3}$$

The energy balance is

$$\frac{\partial}{\partial t}(\rho h)+\frac{\partial}{\partial x}(\rho u h)+\frac{1}{r}\frac{\partial}{\partial}(\rho \upsilon h r)=$$
$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(k\frac{\partial T}{\partial r}r\right)+\frac{\partial}{\partial x}\left(\rho\sum_i D_i h_i\frac{\partial Y_i}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho\sum_i D_i h_i\frac{\partial Y_i}{\partial r}\right)+\rho g u-\sum_i h_i^0\omega_i\,, \tag{4}$$

where:

T - temperature,

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

The standard enthalpy of formation, enthalpy, diffusion coefficient, species mass generation rate, molar weight and mass fraction of species i are respectively denoted as h_i^0, h_i, D_i, ω_i, M_i and Y_i. The fluid viscosity μ, specific heat $c_{p,f}$, and thermal conductivity k are calculated from a mass fraction weighted average of species properties. 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 evaluation of thermal conductivity and molecular viscosity in the mixture.

For each species i, the mass balance am:

$$\frac{\partial(\rho Y_i)}{\partial t}+\frac{\partial(\rho u Y_i)}{\partial x}+\frac{1}{r}\frac{\partial(\rho \upsilon r Y_i)}{\partial r}=\frac{\partial}{\partial x}\left(D_i\frac{\partial(\rho Y_i)}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(D_i r\frac{\partial(\rho Y_i)}{\partial r}\right)+\omega_i\,. \tag{5}$$

The fluid density is calculated using the ideal gas law:

$$\rho=\frac{p}{R_u T\sum_i\frac{Y_i}{M_i}}\,, \tag{6}$$

where R_u is universal gas constant.

The species mass generation rate per unit volume ω_i, can be expressed as:

$$\omega_i=M_i\sum_{k=1}^{K}\omega_{i,k}\,, \tag{7}$$

where $\omega_{i,k}$ is the molar generation rate per unit volume of the species i in kth reaction.

Two global reaction mechanisms were considered. The first one - a one-step reaction mechanism (1-SRM) assumes that C_3H_8 reacts directly with oxygen and leads to CO_2 and H_2O. A reduced one-step propane/air reaction model is given by equations:

$$C_3H_8+5(O_2+3.76N_2)\rightarrow 3CO_2+4H_2O+18.8N_2\,. \tag{8}$$

The second mechanism - a two-step reaction mechanism (2-SRM) is composed of irreversible fuel oxidation step and reversible carbon monoxide oxidation step:

$$C_3H_8 + 3.5O_2 \rightarrow 3CO + 4H_2O\,, \tag{9}$$

$$CO + 0.5O_2 \Leftrightarrow CO_2\,. \tag{10}$$

The rate parameters are taken from Westbrook and Dryer [9]. To solve the conservation equations, a segregated solution solver with an under-relaxation method is used. The pressure was discretized using a "Standard" method. The pressure–velocity coupling was discretized using the "Simple" method. The momentum, species, and energy equations were discretized using a "Second-Order Upwind" approximation. Parameters of reaction mechanisms were chosen according to [8].

Numerical simulations are carried out for 3 mm, 5 mm, 7 mm and 9 mm tubes with isothermal wall conditions (T_{wall} = 298.15 K). Ignition is located in wider tube (opened end) which later evolves into narrow one.

3. Results and discussion

During simulations a flame was initiated near the exit plane of the wider channel by introducing a high-temperature patch in the computational domain. Procedure of determining a limit mixture concentration consisted in observation of flame behaviour after it entered narrow tube. If a flame was able to propagate in it, a mixture concentration was reduced. It was repeated until a difference in equivalence ratio between cases of flame propagation and flame quenching was equalled to 0.01. Characteristics of a limit flame propagating in 3mm tube were evaluated and distribution of temperature, C_3H_8, O_2, CO_2 and H_2O mass fractions for 1-SRM and additionally CO for 2-SRM are plotted as shown in Fig. 2.

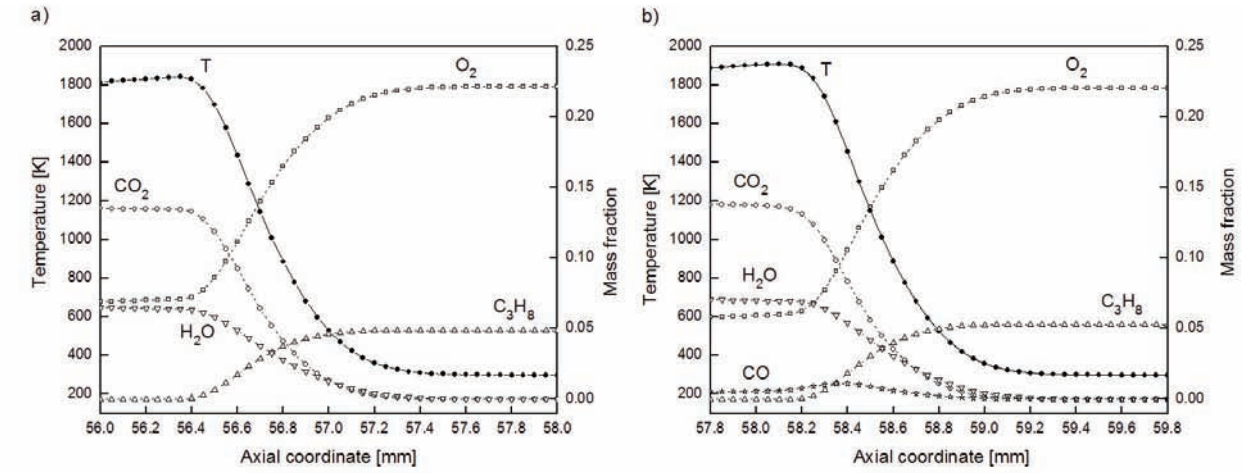

Fig. 2. Flame structure of a limit flames along the axis for 1-SRM (a) and for 2-SRM (b)

Figure 3 shows the structure of flames, which are very close to extinction limit propagating in 3 and 9 mm channels. The upper part of the figure shows normalized reaction rate contours ($\dot{\omega} = \omega_{C_3H_8} / max(\omega_{C_3H_8})$) and the lower part of the figure shows normalized temperature contours defined as $\theta = T/max(T)$.

As can be seen from the temperature distribution, the high-temperature zone ($\theta \geq 0.9$) is at the level of 1.4 mm for 3 mm channel and 4.6 mm for 9 mm channel for 1-RSM. The same parameters for 2-RSM have risen by 6% and 18% respectively.

Quenching diameter as a function of the equivalence ratio is shown in Fig. 4a. As can be seen, using 2-SRM moves a quenching distance for a given tube diameter towards stoichiometric

mixture compares with 1-SRM. This equivalence ratio difference is about 0.08 for flame propagating in 9 mm tube and decreases to 0.07 for 3 mm tube, what is 15% and 8% respectively.

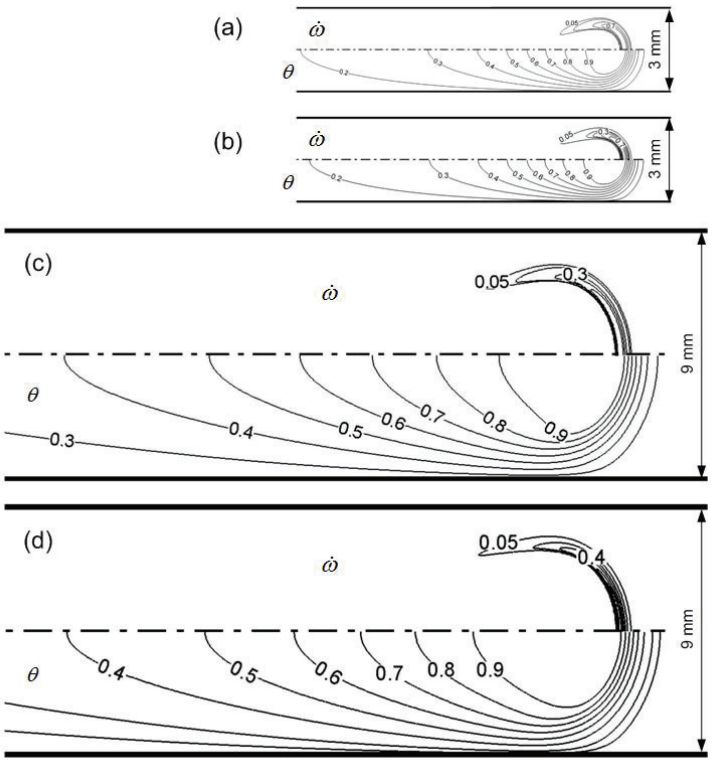

Fig. 3. Normalized reaction rate and temperature contours for limit flames propagating in 3 mm and 9 mm channels for 1-SRM (a), (c) and for 2-SRM (b), (d)

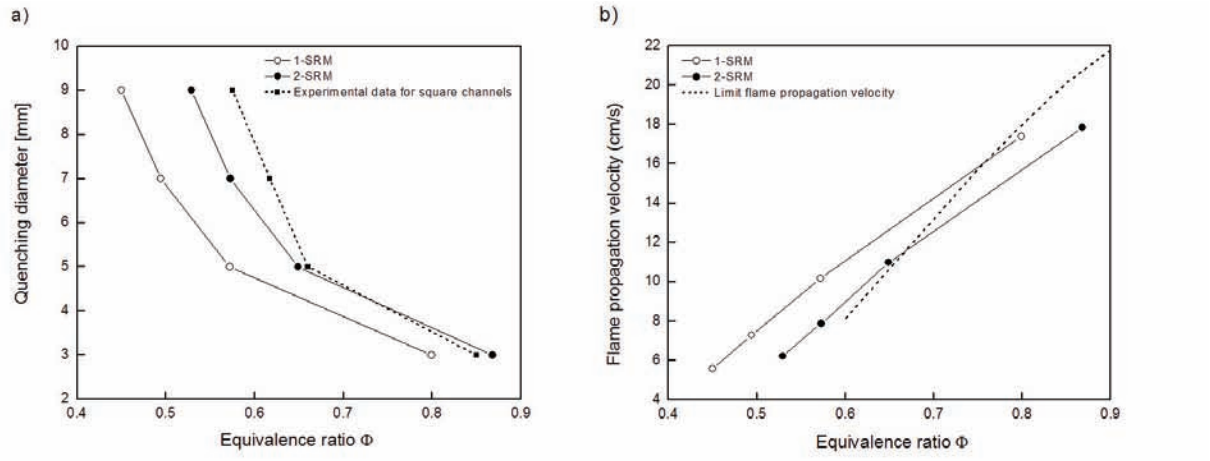

Fig. 4. Quenching diameter (a) and limit flame propagation velocity (b) as a function of equivalence ratio

Due to the lack of experimental data for flames propagating in propane-air mixtures in circular tubes under quenching conditions, it was decided to use similar results of quenching distance as a function of equivalence ratio obtained for square cross-section channels from [3] to make comparison. It can be found a quiet good agreement between experimental data and 2-SRM, especially for $0.65 < \Phi < 0.87$. It is obvious that this comparison can give the answer just about an order of magnitude of the quenching distance, because shape of the cross-section of the channel influences on flame behaviour during its propagation as well on limit mixture concentration. It is expected that quenching distance for flame propagating in square cross-section channel is smaller than in circular tube for a given mixture composition.

Flame propagation velocity as a function of mixture concentration is presented in Fig. 4b. It varies from about 6 cm/s for 9 mm tube diameter to about 17 cm/s for 3 mm. For given mixture concentration 2-SRM gives flame propagation velocity lower than 1-SRM, but from the point of view the tube diameters, difference between these two models is not significant. In order to compare numerical results with experimental values, it is necessary to know limit flame propagation velocity for flames propagating in propane-air mixtures. The aim of the most conducted experimental work is to determine adiabatic laminar propagation velocity, therefore theoretical analysis of flame quenching by the walls explored by Zeldovich [10, 11] is used. He found a relation between laminar propagation velocity at the quenching limit $S_{L,lim}$ and adiabatic laminar propagation velocity S_L:

$$\frac{S_{L,\lim}}{S_L} = e^{-\frac{1}{2}} = 0.61\,. \tag{11}$$

It allows determining values of $S_{L,lim}$. Needed laminar flame propagation velocity under adiabatic conditions was taken from a paper of Vagelopoulos and Egolfopoulos [12]. After comparison it can be stated that 1-SRM model gives results more suitable for mixtures with equivalence ratio close to stoichiometric, while 2-SRM is more appropriate for leaner mixtures.

4. Conclusions

In this consideration, the propagation of lean flames under quenching conditions in propane-air mixtures in circular tubes were investigated numerically using a commercial CFD code ANSYS-Fluent. One and two step reaction mechanisms were considered. The first one assumes that propane reacts directly with oxygen and leads to carbon dioxide and water. The second one predicted existence of carbon monoxide in the reaction zone. Calculated quenching diameters for 2-SRM are moved towards a stoichiometric mixture with reference to 1-SRM. However, quenching distance for both models are of the same order of magnitude as the experimental results obtained for flames propagating in square cross-sections channels. Determined flame propagation velocity shows a very small variation for given tube diameter. If the comparison is prepared for mixture concentration it is visible that 2-SRM gives lower value of flame propagation velocity than 1-SRM. After comparison these values with limit flame propagation velocity it can be stated that 1-SRM model gives results more suitable for mixtures with equivalence ratio close to stoichiometric, while 2-SRM is more appropriate for leaner mixtures.

Acknowledgements

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