Heat Transfer Parameters During Limit Flame Propagation in Small Tubes

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1 Introduction

Zeldovich [1] and Spalding [2] were the first to propose the thermal theory of flame propagation limits in gas mixtures. They shown that flame propagation in narrow channels/tubes is impossible if the characteristic dimension is smaller than the critical value. The combustion limit in channels/tubes is usually characterized by the quenching (critical) value of the Peclet number:

$$Pe_q = \frac{S_L D}{\alpha},$$

Where S_L , D and α are laminar flame propagation velocity, characteristic size of the system and thermal diffusivity, respectively.

Aly and Hermance [3] presented thorough two-dimensional numerical simulations of laminar flame quenching, and a quenching Peclet number value of 60 for stoichiometric mixture was obtained. Their results have also shown that Pe_q increases with decreasing mixture concentration. Numerical exploration of flame propagation in tubes and in parallel plate channels, by Hackert et al. [4], has obtained Peclet number varying from 15 to 60 according to heat loss. Experimental works of Jarosinski et al. [5], which have been conducted in the vertical wedge-shaped channel, showed that Pe_q in a broad range of mixture composition is constant and equals to 42. For rich mixtures it gradually decreases.

A number of study regarding flame propagation inside adiabatic and isothermal ducts have been investigated. Lee and Tsai [6] showed that, in an adiabatic tube, the tulip-shaped flame is a more robust than the mushroom-shaped one. The opposite situation is in a tube with isothermal walls. Kurdyumov et al. [7] have studied Lewis number effect on the flame shape and its propagation velocity. They have found that for Le < 1 flames may propagate in circular tube (with isothermal walls) with higher propagation velocities than those in adiabatic condition. This phenomenon is due to the higher flame curvature near a wall, which leads to higher values of the temperature behind the flame – in spite of the heat losses to the wall.

This short review shows how important for flame propagation under quenching conditions is heat transfer and its real parameters.

In this article, the downward propagation and quenching of lean premixed propane-air flames in small tubes, which are opened at the ignition end and closed at the other, are simulated using a numerical procedure for reacting flow.

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 on the basis of the following assumptions: the system is axisymmetrical and radiation, Soret and Dufour effects are ignored. A scheme of the system is shown in Fig. 1.



Figure 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 to lay along the centerline of the tube. The velocity components u_x and u_r are in x and r directions, respectively. The governing equations can be written as follows:

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_x)}{\partial x} + \frac{1}{r} \frac{\partial (\rho u_r r)}{\partial r} = 0,$$

Momentum equations:

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

$$\frac{\partial(\rho u_r)}{\partial t} + \frac{\partial(\rho u_x u_r)}{\partial x} + \frac{1}{r} \frac{\partial(\rho u_r u_r r)}{\partial r} = -\frac{\partial p}{\partial r} + \frac{\partial}{\partial x} \left(\mu \frac{\partial u_x}{\partial r}\right) - \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{2r\mu}{3} \frac{\partial u_x}{\partial x}\right) + \frac{\partial}{\partial x} \left(\mu \frac{\partial u_r}{\partial x}\right) + \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{4r\mu}{3} \frac{\partial u_r}{\partial r}\right) - \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{2}{3} \mu u_r\right),$$

Energy equation:

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x}(\rho u_{x}h) + \frac{1}{r}\frac{\partial}{\partial}(\rho u_{r}hr) =
\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(k\frac{\partial T}{\partial r}r\right) + \frac{\partial}{\partial x}\left(\rho\sum_{i}D_{i}h_{i}\frac{\partial Y_{i}}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\rho\sum_{i}D_{i}h_{i}\frac{\partial Y_{i}}{\partial r}\right) + \rho gu_{x} - \sum_{i}^{5}h_{i}^{0}\omega_{i}M_{i},
(\omega_{i} = v\omega_{C_{3}H_{8}}),$$

Species equations:

$$\frac{\partial(\rho Y_i)}{\partial t} + \frac{\partial(\rho u_x Y_i)}{\partial x} + \frac{1}{r} \frac{\partial(\rho u_r r Y_i)}{\partial r} = \frac{\partial}{\partial x} \left(D_i \frac{\partial(\rho Y_i)}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(D_i r \frac{\partial(\rho Y_i)}{\partial r} \right) + \omega_i M_i,$$

The fluid density is calculated using the ideal gas law:

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

Where *p* denotes pressure, *g* the gravitational acceleration, *T* temperature, R_u universal gas constant, *h* specific sensible enthalpy ($h = \sum_i Y_i h_i$). The standard enthalpy of formation, enthalpy, diffusion coefficient, reaction rate, molar weight, stoichiometric ratio and mass fraction of a species *i* are respectively denoted as h_i^0 , h_i , D_i , ω_i , M_i , ν 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.

A reduced one-step propane/air reaction model and fuel consumption rate ω_{C3H8} are given by equations:

$$C_{3}H_{8} + 5(O_{2} + 3.76N_{2}) \rightarrow 3CO_{2} + 4H_{2}O + 18.8N_{2},$$

$$\omega_{C3H8} = A \exp\left(-\frac{E_{k}}{RT}\right) [C_{3}H_{8}]^{a} [O_{2}]^{b},$$

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 [8].

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.

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 Flame Propagation in Small Tubes

In this study, freely downward propagation of a premixed flame in an isothermal tube is numerically investigated. Every computational domain consists of two tubes with different diameters

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in order to enable observation of a flame quenching during its entrance into a narrower part. Flames propagating in very lean mixtures are mushroom-shapes in all tube diameters. In wider tubes, as mixture concentration approaches stoichiometric, flames take shape of a tulip. This flame shape transition was described in [4, 6 and 7]. All flames, event those which are tulip-shaped in wider tube became mushroom-shaped after entering into narrower one.

Mixture concentration is recognized as a limit concentration if all heat generated in the reaction is transferred to the wall and it does not cause a flame quenching. If the mixture concentration is below this limit flame is quenched just at the entrance to the tube or after propagating some distance in it. If a tube is sufficiently long, fluid in the post combustion region (where the reactants have been consumed and the reaction stops) would eventually reach wall temperature. Therefore, simulations are curried out until fluid temperature behind a flame does not reach a temperature higher than 1 K over a wall temperature, which corresponds to absence of heat loss to the wall. As an example, calculated heat fluxes for flames propagating and quenching in 3 mm tube are presented in Fig. 2. Curves start at the moment of flame entering a narrow tube. Visible heat flux peaks on the left side (edge of the narrow tube) are a result of almost head-on flame-wall interaction.



Figure 2. Heat flux to the wall for propagating case (a) and quenching one (b). Time interval between curves equals 0.002 s. Equivalences ratio are 0.799 and 0.798, respectively.

Heat flux transferred to the wall sharply decreases at the tube entrance. As flame moves further along the tube it increases and stabilizes with the heat flux maximum fixed at the level of 0.1 MW/m^2 . On the contrary to this case, heat flux of flame quenching does not stabilize, but it decreases as flame is being extinguished. The distance of heat transfer to wall penetration equals about 3 mm.

The length of high temperature gasses *L* differs for various tube diameters. The shortest value is obtained for flame propagating in 3 mm tube diameter (about 28 mm) and the longest is for 9 mm tube -88 mm.

Limit flame propagation velocity for 3 mm tube diameter is equal to 17.4 cm/s. Laminar burning velocity taken from [9] and corresponding to $\Phi = 0.799$ is about 29.2 cm/s. The ratio of these two values gives 0.596 which is close to 0.61 theoretically predicted by Zeldovich [1]. This relation is not constant for all tubes, but increases with tube diameters.

Heat loss to the wall influences flame behavior in the tube, therefore, it is important to calculate heat transfer coefficients for flames propagating under conditions close to quench. It is important to remember that value of heat transfer coefficient is affected by the fact that tube wall is

artificially forced to be isothermal. It can be found using a heat flux between isothermal wall and adjacent fluid. The heat loss to the wall is expressed as:

$$q = h_w (T_{wall} - T_a) = -\lambda \frac{\partial T}{\partial r} \Big|_{wall},$$

where h_w is the interior heat transfer coefficient; T_{wall} is the wall temperature and T_a is the average temperature calculated as the mass-weighted average value from:

$$T_a = \frac{\int_V T\rho dV}{\int_V \rho dV},$$

The volume for which integration is done in a cylinder is limited by the wall of the tube and the length of high temperature region L.

Knowing heat transfer flux to the tube wall, critical interior heat transfer coefficient and its dimensionless form – Nusselt number can be found. Nusselt number is expressed as:

$$Nu = \frac{h_w D}{k},$$

Thermal diffusivity and thermal conductivity are calculated in the same manner as T_a . Heat transfer coefficient and Nusselt number are shown in Fig. 3a and Fig. 3b.



Figure 3. Heat transfer coefficient (a) and Nusselt number (b).

Heat transfer coefficient increases with decreasing of the tube diameters. It rises almost linearly from 42 W/m²/K for the widest tube to 178 W/m²/K for 3 mm tube diameter. Nusselt numbers for these tubes are equal to 13.4 and 18.7 respectively. It suggests that heat loss to the wall is the most intensive during flame propagation in 3 mm tube.

Peclet number is another parameter which is used to describe flames under quenching conditions. Authors in [3] mentioned that it can be calculated using the limit flame propagation velocity, instead of the adiabatic laminar burning velocity. Peclet number based on this definition is equal to $21.7\div22.1$. Improving more Pe_q definition, thermal diffusivity is not calculated for cold mixture, but in the same manner as critical Nusselt number. This choice seems to be more suitable in

our case because takes into account thermal conditions between hot combustion products and cold wall. This modified Pe_q is obtained to be 17.3÷17.8. As one can see, taking into consideration average parameters in combustion products, has en effect on lower value of Pe_q .

It could be very interesting to compare this numerical simulations with experimentally obtained result of flames propagating in wide range of tube diameters. Unfortunately, available results are selective and incomplete.

3 Conclusion

Unsteady premixed flames in narrow tubes with isothermal walls were investigated numerically. Limit mixture concentrations for flames propagating in 3 mm, 5 mm and 7 mm tube diameters were determined. Limit flame propagation velocity for 3 mm tube diameter is close to a value predicted by quenching theory of Zeldovich. There is a difference of this value for others tubes. Explanation of that requires some experimental works, which are being conducted by author.

Calculated heat transfer coefficient for flames propagating under quenching conditions is almost linear function of tube diameters and change from $42 \text{ W/m}^2/\text{K}$ for 9 mm tube to 178 W/m²/K for 3 mm. Nusselt number rises from 13.4 (9 mm) to 18.7 (3 mm).

Two quenching Peclet numbers related to limit flames were determined. The first one is based on limit flame propagation velocity instead of the adiabatic laminar burning velocity. It is equal to $21.7\div22.1$. The second Pe_q was modified by taking into account thermal conditions between hot combustion products and cold wall for calculating thermal diffusivity. Using this definition calculated Pe_q is lower and is equal to $17.3\div17.8$.

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