Variable Density Premixed Thick Flame Propagation in a Microchannel with Heat Conducting Walls

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1 Introduction

The propagation of premixed flames in narrow channels or tubes is an important topic in several areas of combustion research. Emerging technologies such as the development of microscale combustors as a power source for portable devices (e.g. laptops or cell-phones) depend critically on this type of configuration [1]. A large number of papers addressing the issue of flame sustainment and propagation in narrow vessels have appeared in recent years, addressing a range of issues such as heat recirculation, heat loss, catalytic wall effects, Lewis number effects and others (e.g. [2–5]).

Of particular relevance to the current study is the constant density, narrow channel flame propagation studies of Daou and Matalon [6] (for adiabatic walls) and Daou and Matalon [7] (for non-adiabatic walls), as well as the variable density, narrow channel, flame propagation study of Short and Kessler [8] (for adiabatic and non-adiabatic walls). As part of the study in [7], Daou and Matalon examined the behavior of thick flames (the flame width being significantly larger than the channel height) in a non-adiabatic channel, applying a Newton cooling law along the channel wall. The thick flame limit analysis of [6, 7] was extended to variable density flows by Short and Kessler [8]. It was shown that thermal expansion of the hot combustion gases in a narrow channel induce a Poiseuille flow in the channel that has a significant effect on the dynamics of flame propagation.

The current work extends that of Short & Kessler [8] by considering the role played by a conductive solid wall between the channel and an outer insulation layer. The analysis is a formal asymptotic study invoking the thick flame limit (the Peclet number (*Pe*) is small). Heat losses on the outer part of the wall must be restricted to $O(Pe^2)$. We also find that the ratio of the wall height to channel height must scale with the ratio of gas thermal conductivity to wall thermal conductivity. Commonly used microburner wall materials such as quartz (heat conductivity of 1.7×10^{-2} W/cm K, density of 2.2 g/cm³ and a heat capacity of 0.8 J/g K) have a moderately large ratio of wall to gas thermal conductivities (e.g. quartz/air has a thermal conductivity ratio of ~ 100). A 5 mm channel would then require a 50 μ m quartz wall thickness. Other more exotic wall materials could also be considered, e.g. aerogel (thermal conductivities in the range of 4×10^{-5} W/cm K to 3×10^{-4} W/cm K). In principle, with such materials, the height of the wall material could be comparable to the channel height.



Figure 1: Schematic of the channel configuration

2 Model

Channel Flow: Variable density premixed flame propagation in a two-dimensional channel bounded by inert walls is considered (fig. 1). In non-dimensional form, and for a one-step reaction mechanism, the zero Mach number Navier-Stokes equations are

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho(\nabla \cdot \mathbf{u}), \quad \rho \frac{\mathrm{D}u_i}{\mathrm{D}t} = -\nabla p + \frac{1}{Re} \nabla \cdot \tau, \quad \rho T = 1,
\rho \frac{\mathrm{D}T}{\mathrm{D}t} = \frac{1}{Re} \nabla^2 T + Q P e R, \quad \rho \frac{\mathrm{D}Y}{\mathrm{D}t} = \frac{1}{Le P e} \nabla^2 Y - P e R,$$
(1)

for temperature $T (= \tilde{T}/\tilde{T}_0)$, fluid velocity $u_i = (u, v) (= \tilde{u}_i/\tilde{s}_F)$, density $\rho (= \tilde{\rho}/\tilde{\rho}_0)$, pressure $p = ([\tilde{p} - \tilde{p}_r]/\tilde{\rho}_0 \tilde{s}_F^2)$ and fuel mass fraction $Y (= \tilde{Y}/\tilde{Y}_0)$. The temperature scale \tilde{T}_0 is set so that T = 1 in the fresh mixture (where Y = 1), while \tilde{s}_F is the laminar flame speed and $\tilde{\rho}_0 = \tilde{p}_r/(\tilde{R}\tilde{T}_0/\tilde{W})$. The length scale is the half channel height \tilde{a} and the time scale is \tilde{a}/\tilde{s}_F . The nondimensional groups are the Peclet number Pe = PrRe, where Re (Reynolds number) $= \tilde{\rho}_o \tilde{s}_F \tilde{a}/\tilde{\mu}$ and Pr (Prandtl number) $= \tilde{\mu}\tilde{c}_p/\tilde{\lambda}$, the Lewis number $Le = \tilde{\lambda}/\tilde{c}_p\tilde{\rho}\tilde{D}$ and the heat release $Q = \tilde{Q}\tilde{Y}_0/\tilde{c}_p\tilde{T}_0$. Here $\tilde{\mu}$, \tilde{c}_p , \tilde{Q} , \tilde{R} and $\tilde{\lambda}$ are the dimensional dynamic viscosity, specific heat, heat of formation, the gas constant and the thermal conductivity. For the purposes of the present study, they are taken to be constant. The reaction rate is

$$R = D\rho Y \exp(-\theta/T), \tag{2}$$

where the Damköhler number $D = \tilde{D}\tilde{\kappa}_g/\tilde{s}_F^2$ and the activation energy $\theta = \tilde{E}/\tilde{R}\tilde{T}_0$. The thermal diffusivity $\tilde{\kappa}_g = \tilde{\lambda}/\tilde{\rho}_0\tilde{c}_p$, while \tilde{D} and \tilde{E} are the dimensional pre-exponential factor and activation energy.

Wall Thermal Flow: In the wall region, 1 < y < 1 + h, the temperature is determined from the heat diffusion equation

$$Pe\frac{\partial T_s}{\partial t} = \kappa \nabla^2 T_s,\tag{3}$$

assuming constant transport properties, where T_s is the wall temperature. Here $\kappa = \tilde{\kappa}_s/\tilde{\kappa}_g$ is the ratio of the dimensional wall to gas thermal diffusivity, where $\tilde{\kappa}_s = \tilde{\lambda}_s/\tilde{c}_{ps}\tilde{\rho}_s$, with $\tilde{\lambda}_s$, \tilde{c}_{ps} and $\tilde{\rho}_s$ the thermal conductivity, the specific heat, and the density in the solid.

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Boundary conditions: On the outer surface of the wall, y = 1 + h, the Newton cooling law $\partial T_s/\partial y = -Nu(T_s - 1)/\lambda$ is applied, where the Nusselt number $Nu = \tilde{k}\tilde{a}/\tilde{\lambda}_g$ based on a heat transfer coefficient \tilde{k} . Chemically inert and no-slip conditions are imposed on the inner wall, y = 1, where $T_s = T$, $\lambda \partial T_s/\partial y = \partial T/\partial y$, $\partial Y/\partial y = 0$, u = 0, v = 0, with $\lambda = \tilde{\lambda}_s/\tilde{\lambda}_g$ being the ratio of wall to gas thermal conductivities. Channel symmetry flow conditions $\partial T/\partial y = 0$, $\partial Y/\partial y = 0$, u = 0, v = 0, are applied along the centerline (y = 0), thus restricting our solutions to symmetric ones.

3 Small Peclet number approximation

We assume variable density premixed flame propagation in the channel in the limit where the flame thickness is greater than the channel height, or $Pe \rightarrow 0$. The analysis is an extension of the steady theory developed in [8], here describing unsteady flow in the presence of a wall. When $Pe \rightarrow 0$, the axial coordinate, time and the pressure are scaled according to

$$\xi = Pe \, x, \ \tau = Pe \, t, \ \bar{p} = Pe^2 p \tag{4}$$

where ξ , τ and \bar{p} are O(1). With the scales (4), we seek asymptotic solutions to (1) via,

$$T \sim T_0(\xi, \tau) + P e^2 T_1(\xi, y, \tau), \ Y \sim Y_0(\xi, \tau) + P e^2 Y_1(\xi, y, \tau), \tag{5}$$

$$u \sim u_0(\xi, y, \tau), \ \bar{p} \sim \bar{p}_0(\xi, \tau), \ \rho \sim \rho_0(\xi, \tau), \ v \sim Pe \, v_0(\xi, y, \tau),$$
 (6)

which requires the heat loss at the wall (y = 1) to correspond to $\partial T/\partial y = O(Pe^2)$. The derived leading-order axial momentum equation leads to a separable solution for the axial velocity u_0 in channel Poiseuille flow form,

$$u_0(\xi, y, \tau) = \tilde{u}_0(\xi, \tau)(1 - y^2).$$
(7)

The leading-order mass equation can then be subsequently integrated between y = 0 and y = 1, followed by an integration in ξ , to give the axial velocity component \tilde{u}_0 in terms of the leading-order temperature variation T_0 as

$$\tilde{u}_0 = \frac{3T_0}{2} \int_{-\infty}^{\xi} \frac{1}{T_0^2} \frac{\partial T_0}{\partial \tau} d\xi + T_0 u_c.$$
(8)

Compatible velocity boundary conditions are

$$u = u_c (1 - y^2), \ \xi = -\infty.$$
 (9)

With u_c imposed, this corresponds to Poiseuille flow at the inlet to the channel. The downstream end must be open. When the upstream end is closed, $u_c = 0$. On the other hand, when the downstream end of the channel ($\xi \to \infty$, is closed, the upstream end must be open, and \tilde{u}_0 is modified from (8) to

$$\tilde{u}_0 = -\frac{3T_0}{2} \int_{\xi}^{\infty} \frac{1}{T_0^2} \frac{\partial T_0}{\partial \tau} d\xi.$$
(10)

Equations for the leading-order temperature and mass fraction variations T_0 and Y_0 can be obtained by integrating the $O(Pe^2)$ energy and rate equations between y = 0 and y = 1 to give,

$$\frac{1}{T_0}\frac{\partial T_0}{\partial \tau} + \frac{2\tilde{u}_0}{3T_0}\frac{\partial T_0}{\partial \xi} = \frac{\partial^2 T_0}{\partial \xi^2} + \frac{\partial T_1}{\partial y}(\xi, 1, \tau) + QR_0, \tag{11}$$

and

$$\frac{1}{T_0}\frac{\partial Y_0}{\partial \tau} + \frac{2\tilde{u}_0}{3T_0}\frac{\partial Y_0}{\partial \xi} = \frac{1}{Le}\frac{\partial^2 Y_0}{\partial \xi^2} - R_0.$$
(12)

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Thus (8) (or (10)), (11) and (12) are sufficient to determine \tilde{u}_0 , T_0 and Y_0 once $\partial T_1/\partial y$ is determined from the analysis of heat flow in the wall.

With spatial and temporal scales defined by (4), and redefining y such that $\hat{y} = (y-1)/h$, the wall heat equation becomes

$$h^2 P e^2 \frac{\partial T_s}{\partial \tau} = \kappa \left(h^2 P e^2 \frac{\partial^2 T_s}{\partial \xi^2} + \frac{\partial^2 T_s}{\partial \hat{y}^2} \right).$$
(13)

The wall boundary conditions on $\hat{y} = 0$ (y = 1) and on $\hat{y} = 1$ (y = 1 + h) become $\lambda \partial T_s / \partial \hat{y} = hPe^2(\partial T_1/\partial y), \partial T_s/\partial \hat{y} = -hNu(T_s - 1)/\lambda$. For many wall materials, the ratio of thermal conductivities $\lambda \gg 1$, suggesting in such cases a rescaling of λ and Nu, where $\lambda = \hat{\lambda}/h, Nu = Pe^2\hat{N}u$. Thus when $\lambda \gg 1$, the thickness of the wall material is $O(1/\lambda)$. A solution to (13) is now obtained in the form $T_s \sim T_{s0}(\xi, \tau) + h^2 Pe^2 T_{s1}(\xi, y, \tau)$. At $O(h^2 Pe^2)$, equation (13) can be integrated between $\hat{y} = 0$ and $\hat{y} = 1$ to give an evolution equation for T_{s0} :

$$\frac{\partial T_{s0}}{\partial \tau} = \kappa \frac{\partial^2 T_{s0}}{\partial \xi^2} - \frac{\kappa}{\hat{\lambda}} \left(\hat{N}u(T_{s0} - 1) + \frac{\partial T_1}{\partial y} \right).$$
(14)

The temperature condition on the inner wall becomes, $T_{s0}(\xi, \tau) = T_0(\xi, \tau)$, so that by eliminating $\partial T_1/\partial y$ between the channel and wall temperature equations (11) and (14),

$$\left(\frac{1}{T_0} + \frac{\hat{\lambda}}{\kappa}\right)\frac{\partial T_0}{\partial \tau} + \frac{2\tilde{u}_0}{3T_0}\frac{\partial T_0}{\partial \xi} = (1+\hat{\lambda})\frac{\partial^2 T_0}{\partial \xi^2} + QR_0 - \hat{N}u(T_0-1).$$
(15)

Equation (15) for $T_0(\xi, \tau)$ is solved with (12) for Y_0 and (8) for \tilde{u}_0 . The boundary conditions on T_0 and Y_0 are

$$T_0 \to 1, \ Y_0 \to 1, \ \text{as } \xi \to -\infty; \quad \frac{\partial T_0}{\partial \xi} \to 0, \ \frac{\partial Y_0}{\partial \xi} \to 0, \quad \text{as } \xi \to \infty.$$
 (16)

Note that for steady flow and $\hat{\lambda} = 0$ (corresponding to $h \to 0$), (15) reduces to that obtained in [8]. A similar analysis can be conducted for radially-symmetric, variable density flame propagation in a thin-walled circular pipe, and a single system that determines \tilde{u}_0 , T_0 and Y_0 for either channel or pipe flow can be written.

4 Steady and Unsteady Solutions

With U > 0 representing the axial speed of a steady flame propagating to the left in the channel, in a frame of reference traveling with the flame, the steady equations are

$$\rho_0\left(\frac{2}{3}\tilde{u}_0 + U\right) = \left(\frac{2}{3}\tilde{u}_c + U\right) = M, \quad M\frac{\partial Y_0}{\partial \xi} = \frac{1}{Le}\frac{\partial^2 Y_0}{\partial \xi^2} - R_0, \tag{17}$$

$$\left(M\left[1+\frac{\hat{\lambda}}{\kappa}\right]-\frac{2}{3}\frac{\tilde{u}_c\hat{\lambda}}{\kappa}\right)\frac{\partial T_0}{\partial\xi} = (1+\hat{\lambda})\frac{\partial^2 T_0}{\partial\xi^2} + QR_0 - \hat{Nu}(T_0-1).$$
(18)

For finite thickness walls, with $\hat{Nu} = 0$, the product flame temperature becomes

$$T_b = 1 + Q \left(1 + \frac{U\hat{\lambda}}{M\kappa} \right)^{-1} \quad \text{or} \quad T_b = 1 + Q \left(1 + \frac{(1 - 2\tilde{u}_c/3M)\hat{\lambda}}{\kappa} \right)^{-1}, \tag{19}$$

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which depends on the direction and speed of propagation: for U > 0, $T_b < T_{ad}$; for U = 0, $T_b = T_{ad}$ and for U < 0, $T_b > T_{ad}$. When the flame propagates away from a closed end toward an open end, $M = U/T_b$, and the product flame temperature becomes

$$T_b = \frac{1}{2} \left(1 - \frac{\kappa}{\hat{\lambda}} + \sqrt{\left(\frac{\kappa}{\hat{\lambda}} - 1\right)^2 + 4(1+Q)\frac{\kappa}{\hat{\lambda}}} \right), \tag{20}$$

which does not depend on the flame propagation velocity. Further insights into the steady flame structure have been obtained via a large activation energy analysis. Writing $\hat{Nu} = \tilde{Nu}/\theta$, and omitting the details, the main results are

$$M\alpha = \frac{(1+\hat{\lambda})T_b^2(T_{ad}-1)}{(T_b-1)T_{ad}^2}\sqrt{Le}\exp(-\phi_f/2), \ \phi_f = \frac{2(T_b-1)\tilde{N}u(1+\hat{\lambda})}{M^2\alpha^2 T_b^2}.$$
 (21)

where

$$\alpha = 1 + \frac{\lambda U}{\kappa M} = 1 + \frac{\lambda}{\kappa} \left(1 - \frac{2\tilde{u}_c}{3M} \right), \quad T_b = 1 + \frac{Q}{\alpha}, \quad T_{ad} = 1 + Q.$$
(22)

Figure 2 shows some results for the large activation energy analysis, specifically the variation of flame temperature T_b (left) and flame velocity U (right) with axial velocity amplitude \tilde{u}_c of a Poiseuille flow imposed at the channel inlet for Q = 6, Le = 1, $\hat{\lambda} = 1$ and with an adiabatic outer wall. The temperature T_b increases with increases in \tilde{u}_c , while the flame velocity decreases. For U > 0, the flame temperature is below the adiabatic flame temperature $T_{ad} = 1 + Q$, while T_b is higher for larger thermal diffusivities. For U < 0, T_b is greater than T_{ad} , but higher for smaller κ . Figure 3 (left) shows the variation of mass flux M with Nusselt number \tilde{Nu} for Q = 6, Le = 1 and $\hat{\lambda} = 1$ for a range of \tilde{u}_c and diffusivity ratios κ .

We have also studied unsteady pulsating modes of flame propagation obtained from the full system (15), (12) and (8). Figure 3 (right) shows the variation of the reaction rate for a pulsating unstable solution obtained with $D = 12.2786 \times 10^6$, $\theta = 100$, Le = 5, Q = 6, $\tilde{Nu} = 0$, $\hat{\lambda} = 0.1$, $\kappa = 1$ and $\tilde{u}_c = 0$. In summary, the inclusion of a finite thickness wall in a narrow channel has a non-trivial influence on the dynamics of variable density thick flames. In the full paper, a complete characterization of the behavior and influence of variation in the wall thermal parameters on thick flame dynamics will be given both for steady and unsteady flows.

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Figure 2: Variation of flame temperature T_b (left) and flame velocity U (right) with axial velocity amplitude \tilde{u}_c of a Poiseuille flow imposed at the channel inlet for Q = 6, Le = 1, $\hat{\lambda} = 1$ and $\tilde{Nu} = 0$.



Figure 3: (Left) Variation of mass flux M with Nusselt number \tilde{Nu} for Q = 6, Le = 1 and $\hat{\lambda} = 1$ for a range of \tilde{u}_c and diffusivity ratios κ . (Right) Variation of the reaction rate for a pulsating unstable solution obtained with $D = 12.2786 \times 10^6$, $\theta = 100$, Q = 6, Le = 5, $\tilde{Nu} = 0$, $\hat{\lambda} = 0.1$, $\kappa = 1$ and $\tilde{u}_c = 0$.

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