Effects of Gas Compressibility on the Dynamics of Premixed Flames in Long Narrow Channels

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1 Introduction

The propagation of premixed flames in tubes and channels is of significant importance to the understanding of deflagration-to-detonation (DDT) transition in gases [1]. The general perception is that in a confined environment a flame can accelerate into a detonation, but the actual mechanisms leading to flame acceleration remain questionable. Common explanations rely on the onset of turbulence, which leads to wrinkled flames of much larger surface area that propagate at a much higher speed than the laminar flame speed. But even under laminar conditions flame acceleration could result from the combined effects of wall friction and thermal expansion. The resistance exerted on the flow by lateral confinement leads to a highly curved flame near the walls, which is stretched by the large change in density resulting from the heat released during combustion and propagates at increasingly higher speeds. This mechanism has been discussed in our recent publications [2, 3], where we systematically studied the propagation of premixed flames in long narrow channels open at both ends. It was found that in long channels, $L/h \gg 1$ where L is the length of the channel and h its height, the dynamics depend on the ratio of the channel height to the thermal thickness of the flame δ_T , namely on the parameter $a \equiv h/\delta_T$. In relatively narrow channels, $a < a_c$, the flame accelerates through the combustible mixture at a nearly constant rate, that depends on the thermal expansion parameter $\alpha = (T_a - T_u)/T_a$, where T_u is the temperature of the fresh unburned mixture, and T_a the adiabatic flame temperature. For realistic values of α the flame at the end of the channel reaches a speed of approximately six times the laminar flame speed, and the critical value $a_c \approx 5$. In wider channels the flame accelerates first at a constant rate, but after reaching a critical distance that depends primarily on the channel's aspect ratio L/h, it starts accelerating very rapidly in a near-explosion fashion. In these studies, the zero Mach number formulation was adopted, with the Mach number defined as the ratio of the laminar flame speed S_L to the speed of sound c, namely $Ma = S_L/c$. Accordingly, acoustic waves propagate infinitely fast and have no effect on the flame propagation. Related studies by Bychkov et al. [4] and by Demirgok et al. [5] rely on model-type equations for the flame front, and their validity is difficult to assess.

A fast traveling flame generates pressure waves in the unburned gas ahead that tend to preheat the fresh mixture, adding to the heat transferred by conduction that is mainly responsible for its propagation. The pressure waves are generally weak and the question is whether they could, in long enough channels, lead to a significant increase in the flame propagation speed. This scenario is being tested in the present study. In order to isolate compressibility effects from the effects due to confinement observed for $a > a_c$, we have considered here the case $a \ll 1$, in which case the flame propagation speed increases

only mildly and at a nearly-constant rate [2]. A related study was recently carried out by Kagan et al. [6]. Indeed, such narrow channels may not be experimentally accessible. Nevertheless, the adopted simplification enables fundamental understanding of the effects due to compressibility on the flame propagation and allows extracting simple results about the flame dynamics that may be valid beyond the strict range of validity of the model; the asymptotic results for $a \ll 1$ were shown in [3] to remain valid for values as large as $a \approx 5$. Moreover, the channel under consideration may be thought as part of a more general porous media setup consisting of multiple channels separated by thin solid walls of thickness h_w . The ratio $h_w/(h + h_w)$ is then equivalent to the porosity of the media. The periodicity of the model allows focusing on a single channel, and because of the relatively large thermal conductivity of the solid material, the walls may be treated as adiabatic. The more realistic case corresponding to a = O(1), which combines compressibility and effects due to wall resistance will be discussed in a future study.

2 General formulation

A combustible mixture of uniform density ρ_0 and temperature T_0 is contained in a long narrow channel of height h and length L.. When the mixture is ignited at the left end of the channel, x = 0, a premixed flame propagates down the channel towards the right end. The diaphragms containing the mixture in the channel are removed instantaneously upon ignition allowing for the gas exposed to atmospheric pressure to leave the channel freely at both ends. A schematic of the channel configuration is shown on Fig. 1.

The chemical reaction taking place in the channel is modeled by a global irreversible step of the form Fuel + Oxidizer \rightarrow Products. If the reaction is assumed to be first order with respect to each reactant, the mass of fuel consumed per unit volume and unit time



$$\omega_F' \sim (\rho' Y_F / W_F) (\rho' Y_O / W_O) e^{-E/\mathcal{R}T'},$$

where Y_F , Y_O are the mass fractions and



 W_F , W_O the molecular weights of the fuel and oxidizer, respectively, ρ' is the density of the mixture, E is the overall activation energy, \mathcal{R} is the gas constant and T' is the temperature. For lean mixtures the changes in the oxidizer mass fraction during combustion are insignificant and Y_O may be treated as constant; then $\omega'_F = \mathcal{B}\rho'^2 Y e^{-E/\mathcal{R}T'}$ where \mathcal{B} is an appropriately defined pre-exponential factor and the subscript F was removed for simplicity. A similar expression results for the oxidizer consumption rate in a rich mixture, with Y denoting the mass fraction of the oxidizer.

Dimensionless variables are introduced as follows:-

$$\begin{aligned} x &= x'/\delta_T, \quad y &= y'/h, \quad t = S_L t'/\delta_T, \quad u &= u'/S_L, \quad v &= v'/(aS_L), \quad \rho &= \rho'/\rho_u, \\ p &= a^2(p'-p_u)/\rho_0 S_L^2, \quad Y &= Y'/Y_u, \quad \theta &= (T'-T_u)/(T_a-T_u), \end{aligned}$$

where x, y denote the axial and transverse coordinates, u, v the velocity components and p the pressure. The laminar flame speed S_L and the thermal flame thickness $\delta_T = \lambda/\rho_u c_p S_L$ are used as units of velocity and length along the x-direction, and the channel height h is used to nondimensionalize the transverse components with $a = h/\delta_T$; here λ and c_p are the thermal conductivity and specific heat (at constant pressure) of the mixture. The density, temperature, and pressure are made dimensionless using their values in the fresh unburned mixture (denoted by the subscript "u"), such that $p_u = \rho_u \mathcal{R} T_u/\overline{W}$, where \overline{W} is the molecular weight of the mixture (assumed constant). The mass fraction of fuel in the fresh mixture Y_u is used to normalize the mass fraction Y, and the adiabatic flame temperature $T_a = T_u + QY_u/c_p$ is used in the definition of the normalized temperature θ . Finally, we note that the factor a^2 is incorporated in the pressure scaling as appropriate for narrow channels.

Assuming constant transport coefficients, the (dimensionless) governing equations are:

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

$$D\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) = -\frac{1}{a^2}\frac{\partial p}{\partial x} + Pr\left(\frac{1}{a^2}\frac{\partial^2 u}{\partial y^2} + \frac{4}{3}\frac{\partial^2 u}{\partial x^2} + \frac{1}{3}\frac{\partial^2 v}{\partial x\partial y}\right)$$
(2)

$$\rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) = -\frac{1}{a^4}\frac{\partial p}{\partial y} + Pr\left[\frac{1}{a^2}\left(\frac{4}{3}\frac{\partial^2 v}{\partial y^2} + \frac{1}{3}\frac{\partial^2 u}{\partial x\partial y}\right) + \frac{\partial^2 v}{\partial x^2}\right]$$
(3)

$$\rho\left(\frac{\partial\theta}{\partial t} + u\frac{\partial\theta}{\partial x} + v\frac{\partial\theta}{\partial y}\right) - \left(\frac{\partial^2\theta}{\partial x^2} + \frac{1}{a^2}\frac{\partial^2\theta}{\partial y^2}\right) = \frac{\gamma - 1}{\alpha}\Lambda\left(\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial x} + v\frac{\partial p}{\partial y} + Pr\Phi\right) + \omega \quad (4)$$

$$\rho\left(\frac{\partial Y}{\partial t} + u\frac{\partial Y}{\partial x} + v\frac{\partial Y}{\partial y}\right) - \frac{1}{Le}\left(\frac{\partial^2 Y}{\partial x^2} + \frac{1}{a^2}\frac{\partial^2 Y}{\partial y^2}\right) = -\omega,$$
(5)

$$1 + \gamma \Lambda p = \rho (1 + \alpha \theta), \tag{6}$$

where

$$\Phi = \left(\frac{\partial u}{\partial y} + a^2 \frac{\partial v}{\partial x}\right)^2 + a^2 \left[2\left(\frac{\partial u}{\partial x}\right)^2 + 2\left(\frac{\partial v}{\partial y}\right)^2 - \frac{2}{3}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)^2\right]$$

is the viscous dissipation function and $\gamma = c_p/c_v$ is the ratio of specific heats, with c_v the specific heat of the mixture at constant volume. It is convenient in the expression for the reaction rate ω to introduce the large activation energy asymptotic expression for the laminar flame speed $(S_L)_{asp}$, and the adjustment factor $s_L = S_L/(S_L)_{asp}$ that must be numerically calculated for any finite β . Then

$$\omega(Y,\theta) = \frac{\beta^2 (1+\alpha)^2}{2Le \, s_L^2} \, \rho^2 Y \exp\left\{\frac{\beta(\theta-1)}{(1+\alpha\theta)/(\alpha+1)}\right\},\tag{7}$$

where $\beta = E(T_a - T_u)/\mathcal{R}T_a^2$ is the Zel'dovich number ($\beta \gg 1$) with ρ_b the density of the burned gas given by $\rho_b/\rho_u = T_u/T_a$. Values of s_L for β, α considered here were given in [2]. The remaining non-dimensional parameters appearing in these equations include the scaled Mach number $\Lambda = M^2/a^2$, where $M = S_L/c$ is the Mach number based on the laminar flame speed S_L and the speed of sound $c = \sqrt{\gamma p_u/\rho_u}$ at atmospheric pressure, the Prandtl number $Pr = \mu c_p/\lambda$ with μ the viscosity of the mixture, and the Lewis number $Le = \lambda/\rho_u c_p \mathcal{D}$, with \mathcal{D} the (fuel-inert) mass diffusivity. Setting $\Lambda = 0$ we recover the zero-mach number equations.

Assuming symmetry, it is sufficient to specify boundary conditions along the centerline of the channel y = 1/2 and at one of the walls, y = 0 say, as follows:

at
$$y = 1/2$$
: $v = \partial u/\partial y = \partial \theta/\partial y = \partial Y/\partial y = 0,$ (8)

at
$$y = 0$$
: $u = v = \partial Y / \partial y = \partial \theta / \partial y = 0$. (9)

The boundary conditions at the two ends are:

$$\underline{\operatorname{at} \ x = 0, \ell}: \quad p = v = \partial u / \partial x = \partial \theta / \partial x = \partial Y / \partial x = 0 \tag{10}$$

where $\ell = L/\delta_T$. These conditions are invariably appropriate when the flame is not within an $O(\delta_T)$ distance from either end, with appropriate modifications required otherwise; these however will have a negligible effects on the overall flame propagation for $\ell \gg 1$.

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3 Narrow channels

We consider now the case of a narrow channel $a \ll 1$, and expand all variables in power series of a^2 , i.e., in the form $f = f_0 + a^2 f_1 + \ldots$ To leading order, Eqs (4)-(5) simplify $\partial^2 \theta_0 / \partial y^2 = 0$, $\partial^2 Y_0 / \partial y^2 = 0$ which, when integrated from y = 0 to y = 1/2 and using the appropriate boundary conditions yield $\theta_0 = \theta_0(x, t)$ and $Y_0 = Y_0(x, t)$. Variations in the mixture properties across the narrow channel are negligibly small, and θ_0, Y_0 , which represent the mean (in the transverse direction) temperature and the mass fraction, vary only with x and t. The momentum equations (2)-(3) reduce, to leading order, to

$$\frac{\partial p_0}{\partial y} = 0, \quad \frac{\partial p_0}{\partial x} = Pr \frac{\partial^2 u_0}{\partial y^2};$$
(11)

the first implies that $p_0 = p_0(x, t)$, and permits a direct integration of the second equation which, when using the boundary conditions (8) and (9) yields $u_0 = 6Uy(1 - y)$, where U is the mean axial velocity in the channel and

$$\partial \tilde{p}_0 / \partial x = -U(x, t).$$
 (12)

for the reduced pressure $\tilde{p}_0 = p_0/12Pr$. The continuity equation can now be integrated to give

$$\rho_0 v_0 = -\left[\frac{\partial \rho_0}{\partial t}y + \frac{\partial (\rho_0 U)}{\partial x}(3y^2 - 2y^3)\right]$$

where $v_0 = 0$ at y = 0 has been satisfied. The condition $v_0 = 0$ at y = 1/2 then yields

$$\frac{\partial \rho_0}{\partial t} + \frac{\partial (\rho_0 U)}{\partial x} = 0.$$
(13)

Note that the flow field (u_0, v_0) depends on the density ρ_0 and hence on the temperature θ_0 and mass fraction Y_0 which, at this stage are undetermined.

Focusing on equations (4)-(5), we now proceed to the next order in a^2 , and find

$$\frac{\partial^2 \theta_1}{\partial y^2} = \rho_0 \frac{\partial \theta_0}{\partial t} + \rho_0 U \frac{\partial \theta_0}{\partial x} - \frac{\partial^2 \theta_0}{\partial x^2} - \frac{\gamma - 1}{\alpha} \Pi \left[\frac{\partial \tilde{p}_0}{\partial t} + u_0 \frac{\partial \tilde{p}_0}{\partial x} + \frac{1}{12} \left(\frac{\partial u_0}{\partial y} \right)^2 \right] - \omega(\theta_0, Y_0)$$
(14)

$$\frac{1}{Le}\frac{\partial^2 Y_1}{\partial y^2} = \rho_0 \frac{\partial Y_0}{\partial t} + \rho_0 U \frac{\partial Y_0}{\partial x} - \frac{1}{Le}\frac{\partial^2 Y_0}{\partial x^2} + \omega(\theta_0, Y_0)$$
(15)

where $\Pi \equiv 12Pr\Lambda$. Integrating equations (14)-(15) from y = 0 to y = 1/2, and using (12) and (8)-(9), yields

$$\rho_0 \frac{\partial \theta_0}{\partial t} + \rho_0 U \frac{\partial \theta_0}{\partial x} - \frac{\partial^2 \theta_0}{\partial x^2} = \frac{\gamma - 1}{\alpha} \Pi \frac{\partial \tilde{p}_0}{\partial t} + \omega(Y_0, \theta_0), \tag{16}$$

$$\rho_0 \frac{\partial Y_0}{\partial t} + \rho_0 U \frac{\partial Y_0}{\partial x} - \frac{1}{Le} \frac{\partial^2 Y_0}{\partial x^2} = -\omega(Y_0, \theta_0)$$
(17)

Adding Equ. (13) multiplied by $(1+\alpha)\theta$ to Equ. (16) multiplied by α and using the equation of state (6), one obtains an equation for the pressure \tilde{p}_0 , namely

$$\Pi \frac{\partial \tilde{p}_0}{\partial t} - \frac{\partial}{\partial x} \left[(1 + \gamma \Pi \tilde{p}_0) \frac{\partial \tilde{p}_0}{\partial x} \right] = \alpha \left(\frac{\partial^2 \theta_0}{\partial x^2} + \omega \right), \tag{18}$$

which was first derived in [6]. Thus, for narrow channels, the problem reduces to solving the initial value problem consisting of equations (16)-(17) for the temperature and mass fraction, equation (18) for the pressure and (12) for U, with the density given by the equation of state (6). These equations are to be solved for $0 < x < \ell$ subject to the boundary conditions (10). The flame position x_f is defined below as the position x at time t where the reaction rate ω reaches its maximum value.

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4 Numerical results

Numerical results of the initial value problem were obtained using a second-order, three-points difference scheme for the spatial derivatives with typical resolution of $\Delta x = 0.02 \div 0.05$, and a first-order approximation for time derivatives with a time step $\Delta t = 10^{-6} \div 10^{-7}$. No significant differences were found in the results when Δx and Δt were halved. The corresponding temperature and mass fraction equations were solved using an explicit method while the pressure equation was solved implicitly using the Thomas algorithm. The initial conditions imposed were in the form of a hot spot located near x = 0; the extent of the hot spot was found to have practically no effect on the flame dynamics.



Figure 2: Temperature history in a channel of length $\ell = 200$ for two values of Π .



Figure 3: Pressure history in a channel of length $\ell = 200$ for two values of Π .

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Of primary interest in this study is the parameter Π , which is proportional to the representative Mach number and is a measure of compressibility effects on flame dynamics. To illustrate the importance of compressibility effects we present in Figs. 2 and 3 temperature and pressure profiles at increasing times for the representative value $\Pi = 0.01$ as compared to the profiles for $\Pi = 0$, where compressibility effects are absent. The main effect of compressibility is preheating the fresh mixture, as is evident in Fig. 2(b), and the subsequent increase in flame temperature and propagation speed. The pressure gradients that result from lateral confinement are significantly larger when compressibility effects are present, as shown in Fig. 3(b), adding significant thrust that pushes the fresh mixture and draws the flame towards the right end of the channel. Figure 4 shows the time history of the propagation speed \dot{x}_f calculated for $\ell = 200$ and several values of Π . For $\Pi = 0$, the flame accelerates towards the end of the channel at a nearly constant rate, with $\dot{x}_f = \exp(\alpha t/\ell)$ shown as the open circles in the figure, as discussed in [2]. As Π increases, the flame accelerates extremely fast, in a near-explosion fashion, within a relatively short distance. Finally, it should be noted that for a given mixture and chemistry, determined by the values of β , α and γ , the flame propagation in a long narrow channels is governed solely by the parameter Π .



Figure 4: Propagation speed calculated for several values of Π with $\ell = 200$; the open circles for $\Pi = 0$ correspond to the asymptotic formula derived in [2].

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