# Transient inwardly propagating Hydrogen-Air flames subject to pressure fluctuations and stretch

Nadeem A. Malik<sup>1,2</sup>

<sup>1</sup>Queen Mary University of London, School of Engineering and Materials Science,

Mile End Road, London E1 4NS, England

<sup>2</sup>Imperial College London, Department of Mechanical Engineering,

Exhibition Road, London SW7 2AZ, England

## 1 Introduction

The availability of fast computers and the development of numerical software has made it possible to simulate combustion processes with full pressure velocity coupling in compressible flow coupled also to comprehensive chemical mechanisms. Increasingly detailed studies are now possible in areas of combustion which were previously un-explored due to the difficulties associated with experiments and the limitations of numerical methods. An area of especial importance is the regime of relatively high Karlovich number,  $Ka = t_L/t_v \ge 1$ , Ka is the ratio of the chemical time scale to the convective (turbulent) time scale. In this limit, the convective fluctuations can penetrate inside the internal structure of the flame thus disturbing the steady laminar flame profile and the system is then essentially unsteady. Little is known of the flame response in this limit, and yet it is of fundamental and practical importance because most combustion occurs under turbulent conditions such as in internal combustion engines when the smaller convective scales are able to penetrate inside the flame kernel. To date, most models of turbulent flames often assume that the turbulent flame front consists of a collection of laminar flamelets so that the steady laminar flame structure is assumed undistrubed. Clearly, such an assumption cannot be valid at all times.

Previous studies have often made simplifying assumptions, such as fluctuations in only one physical variable, or 1-step chemistry, see [1]–[4] and computational studies are relatively few, [5]-[7]. These type of studies focus on particular effects in isolation. However, there is a need to look at the complexity of transient effects in its entirity as this is probably more common. In a recent study Malik & Lindstedt [8] explored the response of premixed hydrogen-air planar and outwardly propagating cylindrical and spherical flames subject to pressure oscillations in moderately inhomogeneous mixtures. They used an implicit Eulerian method in a fully coupled compressible flow system with comprehensive H2-Air chemical mechanism. They found that different species responded differently to the pressure oscillations depending upon the thickness of their respective profiles relative to the scale of the physical disturbance. Some evidence of a time lag or 'memory effect' between fuel consumption and the rate of heat relase was observed, and large varuations in the streched flame speed was observed as pressure induced strain rates impacted upon the reaction layer.

Correspondence to : n.a.malik@qmul.ac.uk

A study of methane-air, [9] (also ICDERS 2009), shows similar trends with respect to the differing response of species depending upon their thickness with respect to the wavelength of the physical oscillation; however the timescale of diffusive-reacting coupling is much longer and this is manifested in the much longer relaxation times. This is especially important as hydrocarbon flames are the most common type of flames in industrial applications.

Inwardly propagating spherical flames are important for two reasons. First, experimentally they are difficult to produce and little data is available; exceptions are [5]-[7] under various conditions. Baillot et al [6] produced small spherical bubbles of methane-air about 1 mm diameter which have very high curvature. Numerical simulations of imploding flames are also scarce; Bradley [5] investigated the methane-air system using a a simplified 4 step mechanism and a simplied set of balance equations in which the momentum equation was neglected under the assumption that pressure gradients were negligable.

Second, inwardly propagating flames are not subject to strain effects due to the zero velocity ahead of the flame. Thus, stretch is due to the curavture alone and so the effects of curvature can be studied in isolation. More precisely, stretch is given by the general expression [4]

$$\kappa = (-n \otimes n : \nabla u + \nabla \cdot u) + U_n(\nabla \cdot n) \tag{1}$$

where the fist term is that due to the strain, n is the unit vector normal to the flame front pointing towards the unburnt side, u is the local flow velocity, and  $U_n$  is the burning velocity normal to the flame surface. Relative to the unburned mixture in the limit of thin flames, such as wrinkled flames where  $\delta/\Lambda \ll 1$  and  $\Lambda$  is the length scale of wrinkling, we have a general linear expression for the flame speed deficit [10], [11]

$$U_L - U_n = L\kappa \tag{2}$$

where L is a Markstein length which depends of the strain and curvature.

For inwardly propagating flames, the strain term is absent and the curvature is negative, and we obtain

$$U_L - U_n = L_c U_n \nabla \cdot n = -L_c \frac{2U_n}{r_u}.$$
(3)

If  $L_c > 0$  then  $U_n < U_L$ , that is the negatively stretched burning speed is slower than the unstretched burning speed. On the other hand, if  $L_c < 0$  then  $U_n > U_L$  and the burning speed is enhanced.

#### 2 Aims

In this paper, stochiometric hydrogen-air flames are studied in the context of *inwardly* propagating cylindrical and spherical flames. The advantage of inwardly propagating flames is that the unburnt velocity is zero and thu the strain rate due to the geommetry is also zero. The flame stretch is then due to the curvature alone plus the local strain induced by the local pressure fluctuations.

A question of general interest is how stretch (curvature) affects other properties of the flame, not just the stretched laminar flame velocity. The main aim of this work is to explore the coupling of the thermochemical flame structure to thermoacoustic oscillations in the context of inhomogeneous fuel distributions and for different levels of negative curvature.

#### 3 Method

The current work features an Eulerian method, described in [8]. The balance equations of mass, momentum, energy and chemical species, together with the state equation for ideal gas, are solved in an implicit framework on a staggered grid arrangement. The diffusive fluxes include the Soret thermal–diffusion for light species (H and  $H_2$ ), and the effects of non-zero Lewis number for each species. The chemistry is modelled as a comprehensive system of elementary reactions, featuring 9 species and 30 reactions, see table 1 for details. Thermodynamic data were computed using JANAF polynomials.

Transmissive boundary conditions were imposed on the gas velocity at the open boundaries; and acoustic pressure waves were reflected back at the open ends of the domains. For the curved flames, u = 0 at r = 0.

The balance equations are solved implicitly using a fractional step finite volume method with central differencing and a second order van Leer flux limiter for high cell Peclet number. The energy equation is solved first, and then the momentum and continuity equations are solved using a PISO-type method by setting up a Poisson equation for the pressure field. Finally, all the species mass fractions are solved simultaneously using a Newton-Raphson linearisation of the chemical source term, which yields a block tri-diagonal system of algebraic equations. The process is iterated until the full equation set is converged before the time-step is advanced. The solution method is second order accurate in both time and space. The implicit nature of the numerical scheme provides the required stability to resolve all the spatial and time scales inside the flame kernel.

The domain size was chosen to be L = 400mm which was found to produce pressure oscillations in the required frequency range 100 - 1000Hz: an initial set of pressure ramps in the domain were allowed to diffuse, convect and reflect off the domain boundaries until a they reach a state of quasi– random oscillations with rms fluctuations  $p' \sim 1 - 2\%$  of atmospheric pressure. The fuel inhomogeneity was then introduced as a sinusoidal oscillation cycle in the equivalence ratio just ahead of the flame front at time t = 0s, viz  $\phi(r) = 1.0 + A_{\phi} \sin(2\pi r/\lambda_{\phi})$ , where  $\lambda_{\phi}$  is the lengthscale of variation  $A_{\phi}$  is the initial amplitude. Four cases of moderate inhomogeneity  $A_{\phi} \ll 1$  for each flame were consider,  $A_{\phi} = -0.2, -0.1, 0.1, 0.2.$ 

#### 4 Results & Discussion

Figure 1 shows the profiles of four selected species, H, OH, HO2 and O. As in [8] Figure 10 the thin HO2-profile is not penetrated by the pressure fluctuations and is affected only in its peak amplitude which adjusts to the local fluctuations. On the other hand, the thick OH-profile is disturbed across its whole length. The H-profile is an in between case.

Figure 2 shows the laminar flame speed  $U_L$  as the flames propagate through the equivalence ratio oscillation cycle: the sinusoidal variation in the mean is evident, as well as the local variations due to the pressure fluctuations.  $U_L$  is computed directly as the integral of the fuel rate of reaction across the domain, and normalised by a factor of  $\rho_u(Y_F^u - Y_F^b) - u$  refers to unburnt quantities, and b refers to burnt quantities. Although the plots in Figure 2 are similar to those for the *outwardly* propagating curved flames as observed in Figures 5(b) and 5(c) in [8], the relaxation times here for the *inwardly* propagating curved flames are longer by about 50%. We have defined the flame relaxation time  $\tau_R$ , [8], as the time that the flame speed-curves in Fig. 2 first cross-over. This is a quantity that provides a measure of the time scale of unsteady processes in the system. We also define a non-dimensional relaxion number  $n_R$ ,

$$n_R = \frac{\tau_R}{t_L} \tag{4}$$

which is the ratio of the relaxation time to the flame time scale which we define as  $t_L \sim \delta_L/U_L$ , where  $\delta_L \sim D_{th}/U_L$  is the laminar flame thickness and  $D_{th}$  is the thermal diffusivity, all quantities being evaluated in the fresh gases. Thus,  $n_R$  contains information about the balance of the unsteady processes in the system. A small value of  $n_R$  indicates that scalar diffusional processes are fatser than thermochemical heat transport.

The lack of mean strain ahead of inwardly propagating flame and the negative curvature appear to alter the balance of heat and mass transport processess such that flame propagation is reduced with respect to the rate of scalar (fuel equivalence ratio) dissipation. This is consistent with the expression



Figure 1: Mole-fractions of indicated species against time and radius. Cylindrical flame with  $A_{\phi} = 0.2$ 

for the flame speed  $U_n$  in equation (3) if the Markstein length is negative, and hence  $U_n < U_L$ . (But note that Bradley [5] found that  $L_c$  was small but positive.)

In [8] and [9] Malik & and Lindstedt have shown that the flame relaxion number  $n_R$  in outwardly propagating methane-air flames are much larger than in outwardly propagating H2-air flames. The mechanism there is due to the natural differences in H2-air and CH4-air flame thicknesses and time scales.

However, here, we are comparing the same H2-air flame, one propagating outward,[8], and the other in this paper propagating inward. Therefore, the increase in  $n_R$  by 50% must be due to the flow and geometric configurations alone. The balance of kinetic and transport processes like differential diffusion and Soret thermal diffusion must have been altered through their coupling with the curavture and perhaps also with the local the pressure fluctuations.

Thus, while there are similarities, there are also significant differences in the responses of inwardly and outwardly propagting H2-air flames. By the ICDERS 2009 conference, a more detailed analysis of these and other results will be presented.



Figure 2: Laminar flame speed against time. Left: Cylindrical flame, Right: Spherical flame

## References

- Candel, S. (2002) Combustion Dynamics and Control: Progress and Challenges, Proc. Combust. Inst., 29, 1-28.
- [2] Lieuwen, T. (2005) Nonlinear Kinematic Response of Premixed Flames to Harmonic Velocity Disturbances. Proc. Combust. Inst., 30, 1725–1732.
- [3] Teerling, O.J., McIntosh, A.C., Brindley, J. and Tam, V.H.Y. (2005) Premixed Flame Response to Oscillatory Pressure Waves. Proc. Combust. Inst., 30, 1733-1740.
- [4] Candel S.M. & Poinsot T.J. (1990) Combust. Sci. Tech., 70:1, 176–198. (1990)
- [5] Bradley, D., Gaskell, P. and Gu, X.J. (1996) Burning Velocities, Markstein Lengths and Flame Quenching in Spherical Ethane–air Flames: A Computational Study. *Combust. Flame*, 104, 176–198.
- [6] Baillot F., Durox D., & Demare D., (2002) Experiments On Imploding spherical flames: effects of curvature. Proc. Combust. Inst., 29, 1453–1460.
- [7] Groot G.R.A. & De Goey L.P.H. (2002) A Computational study on propagating spherical and cylindrical premixed flames. Proc. Combust. Inst., 29, 1445–1451.
- [8] Malik N.A. & lindstedt R.P. (2009a) The response of transient premixed flames to stretch and simultaneous pressure and equivalence ratio fluctuations Under review, Combustion, Science & Technology.
- [9] Malik N.A. & lindstedt R.P. (2009b) The response of transient premixed methane-air flames to stretch and simultaneous pressure and equivalence ratio fluctuations *Proceedings*, *ICDERS 2009*.
- [10] Clavin, P. & Williams, F.A., J. Fluid Mech. 116:251 (1982)
- [11] Clavin, P., Prog, Ener. Combust. Sci. 11:1 (1985)
- [12] Sun, H., Yang, S.I., Jomaas, G. and Law, C.K. (2007) High-pressure Laminar Flame Speeds and Kinetic Modeling of Carbon Monoxide/Hydrogen Combustion. Proc. Combust. Inst., 31, 439–446.

Number	Reaction		$A^{\mathrm{a}}$	$n^{\mathrm{a}}$	$E^{\mathbf{a}}$	
1	$H + O_2 \rightleftharpoons O + OH$		$6.73E{+}12$	-0.50	69.75	
2	$O + H_2 \rightleftharpoons H + OH^b$		5.08E + 01	2.67	26.33	
3	$H_2 + OH \rightleftharpoons H_2O + H$		2.17E + 05	1.52	14.47	
4	$Oh + OH \rightleftharpoons O + H_2O$		3.35E + 01	2.42	-8.06	
5	$H_2 + M \rightleftharpoons H + H + M^c$		$2.23E{+}11$	0	40.196	
	$H_2 + H_2 \rightleftharpoons H + H + H_2$		$9.03E{+}11$	0	40.196	
	$H_2 + N_2 \rightleftharpoons H + H + N_2$		$4.58E{+}16$	-1.40	43.681	
	$H_2 + H_2O \rightleftharpoons H + H + H_2O$		$8.43E{+}16$	-1.10	43.681	
6	$O + O + M \rightleftharpoons O_2 + M^d$		6.16E + 09	-0.5	0.0	
7	$O + H + M \rightleftharpoons OH + M^d$		$4.71E{+}12$	-1.0	0.0	
8	$\rm H + OH + M \rightleftharpoons H_2O + M^e$		$2.21E{+}16$	-2.0	0.0	
9	$O_2 + H (+ M) \rightleftharpoons HO_2 (+ M)^f$	$k_0$	$2.65E{+}13$	-1.30	0.0	
		$k_{\infty}$	4.65E + 09	0.4	0.0	
	$O_2 + H (+ H_2O) \rightleftharpoons HO_2 (+ H_2O)^g$	$k_0$	$3.63E{+}13$	-1.00	0.0	
		$k_{\infty}$	4.65E + 09	0.4	0.0	
10	$H_2 + O_2 \rightleftharpoons HO_2 + H$		7.40E + 02	2.43	223.85	
11	$\mathrm{HO}_2 + \mathrm{H} \rightleftharpoons \mathrm{OH} + \mathrm{OH}$		$6.00E{+}10$	0	1.23	
12	$HO_2 + O \rightleftharpoons OH + O_2$		$1.63E{+}10$	0	-1.86	
13	$\mathrm{HO}_2 + \mathrm{OH} \rightleftharpoons \mathrm{H}_2\mathrm{O} + \mathrm{O}_2^{\mathrm{b}}$		$1.00E{+}10$	0	0.00	
			5.80E + 10	0	16.63	
14	$\mathrm{HO}_2 + \mathrm{HO}_2 \rightleftharpoons \mathrm{H}_2\mathrm{O}_2 + \mathrm{O}_2^{\mathrm{b}}$		$4.20E{+}11$	0	50.133	
			1.30E + 08	0	-6.817	
15	$H_2O_2 (+ M) \rightleftharpoons OH + OH (+ M)^h$	$k_0$	$1.2E{+}14$	0	190.37	
		$k_{\infty}$	$3.00E{+}14$	0	202.84	
16	$H_2O_2 + H \rightleftharpoons H_2O + OH$		$1.02E{+}10$	0	14.96	
17	$H_2O_2 + H \rightleftharpoons H_2 + HO_2$		1.69E + 09	0	15.71	
18	$H_2O_2 + O \rightleftharpoons OH + HO_2$		8.43E + 08	0	16.61	
19	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2^{b}$		$1.70E{+}15$	0	123.05	
			2.00E + 09	0	1.79	
20	$HO_2 + H \rightleftharpoons H_2O + O$		1.44E + 09	0	0	

**Table 1.** Detailed  $H_2/O_2$  Reaction Mechanism with rate coefficients in the form  $k = AT^n exp(-E/RT)^a$  from Sun et al. (2007). The rate proposed by Sutherland et al. (1986) was used for reaction (2).

<sup>a</sup>Units are kmole, m<sup>3</sup>, s, K and KJ/mole.

<sup>b</sup>Reactions (13), (14) and (19) are expressed as the sum of the two rate expressions.

 $^{\rm c}{\rm Chaperon}$  efficiencies are 0.0 for  ${\rm H}_2,\,{\rm H}_2{\rm O},\,{\rm N}_2$  and 1.0 for all other species.

 $^{\rm d}$ Chaperon efficiencies are 2.5 for H<sub>2</sub>, 12.0 for H<sub>2</sub>O and 1.0 for all other species.

<sup>e</sup>Chaperon efficiencies are 2.5 for  $H_2$ , 6.39 for  $H_2O$  and 1.0 for all other species.

<sup>f</sup>Troe parameter is  $F_c=0.57$ . Chaperon efficiencies: 1.49 for  $H_2$ , 0.0 for  $H_2O$  and 1.0 for other species.

<sup>g</sup>Troe parameter is  $F_c=0.81$ . Chaperon efficiencies: 1.0 for  $H_2O$  and 0.0 for other species.

<sup>h</sup>Troe parameter is  $F_c=0.50$ . Chaperon efficiencies: 2.5 for  $H_2$ , 12.0 for  $H_2O$  and 1.0 for other species.