The response of transient inhomogeneous methane-air flames subject to pressure fluctuations and stretch

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1 Introduction

In the limit of high Karlovitz (Ka) numbers $(Ka = t_c/t_v \gg 1)$, where Ka is the ratio of the chemical timescale (t_c) to the convective (turbulent) timescale (t_v), fluctuations can penetrate the internal flame structure and perturb the quasi–steady propagation mode and cause the system to become essentially unsteady. This regime is of fundamental and practical importance because most combustion occurs under turbulent conditions such as in internal combustion engines where, depending on the conidtions, the smaller convective eddies are able to penetrate inside the flame kernel.

The recent progress in computer technology makes it possible to explore this important regime of combustion in detail. Malik & Lindstedt [1] have explored the response of outwardly propagating hydrogen–air flames to simultaneous pressure–oscillations and stretch and Malik [2] has studied the same system for inwardly propagating hydrogen–air flames. The method used in both these studies was an implicit Eulerian method with full pressure–velocity coupling in compressible flow and coupled to comprehensive chemical mechanisms. The method has the capability of resolving all the convective and chemical length and time scales, which is essential for resolving these highly stiff chemically reacting flows.

Past investigations [1] found that pressure fluctuations in the range 100–1000 Hz coupled to the flame, and that different species responded differently to the pressure oscillations depending upon the relative thickness of their respective reaction zones to the length scale of the fuel distribution. Some evidence of a time lag or 'memory effect' between fuel consumption and the rate of heat relase was observed. Stretch also appeared to play an important role in determining the flame response.

2 Aims

In the current work, stoichiometric methane–air flames are studied in the context of planar flames and *outwardly* propagating cylindrical and spherical flames in order to shed more light on the coupling of the

thermochemical flame structure to thermoacoustic oscillations in the context of an inhomogeneous fuel distribution and for different levels of curvature and stretch. What is the balance of transport processes under the impact of stretch and fuel inhomogeneity in different types of flames? What is the underlying phsyics of thermoacoustic interactions when the flame kernel is disturbed.

The comparison between hydrogen–air flames and hydrocarbon–air systems is very important in combustion research, especially at a practical level because the latter are the most prevalent flame types in industry. There are also important differences in molecular transport properties because hydrogen is light and therefore has a much higher thermal diffusion component in its heat and mass transport balance, which could play an important role in the flame response to physical disturbances.

3   Method

The current work features an Eulerian method [1] in which 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 governing equations and models for the various fluxes are given in [1]. The diffusive fluxes include Soret thermal–diffusion for light species (H and H_2). The chemistry is modelled as a comprehensive system of elementary reactions whose rates are given by,

$$\dot{R}_k \quad = \quad \sum_{j=1}^{N_r}(\nu_{kj}^{''} - \nu_{kj}^{'}) \left[k_j^f \prod_{l=1}^{N_s} \phi_l^{\nu_{jl}^{'}} - k_j^r \prod_{l=1}^{N_s} \phi_l^{\nu_{jl}^{''}} \right] \tag{1}$$

where ϕ_l is the molar concentration of the lth chemical species, and $\nu^{'}$ and $\nu^{''}$ are the stoichiometric coefficients of reactants and products respectively. The forward reaction rate constant in reaction number j is given by Arrhenius' law,

$$k_j^f \quad = \quad A_j T_j^{\beta} \exp(-\Delta E_j/RT) \tag{2}$$

where the constants A, β and the energy barrier ΔE_j, for the hydrogen sub-system were obtained from Sun et al [3]. The complete chemistry features 30 species (containing up to 2 carbon atoms) and 148 reactions with the hydrocarbon part as outlined by Lindstedt [4]. The rate constant for the $O + H_2 = OH + H$ reaction was altered to the original CEC recommendation – see [1] for details. Thermodynamic data were computed using JANAF polynomials.

Transmissive boundary conditions were imposed on the 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 were 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 was solved first, and then the momentum and continuity equations were solved using a PISO–type method by setting up a Poisson equation for the pressure field. Finally, all the species mass fractions were solved simultaneously using a Newton–Raphson linearisation of the chemical source term, which yields a block tri–diagonal system of algebraic equations. The process was repeated until the full equation set was 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.

4   Results & Discussion

Random acoustic pressure waves with frequencies in the range 100-1000 Hz were set up inside a domain size of $L = 400$ mm by allowing an initial set of pressure ramps in the domain to diffuse, convect and reflect back off the open ends of the domain until a quasi–steady state of pressure fluctuations with $p' \sim 1 - 2\%$ of atmospheric pressure was obtained 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 λ_ϕ is the lengthscale of variation A_ϕ is the initial amplitude. Four cases of moderate inhomogeneity $A_\phi \ll 1$ for each flame were consider, $A_\phi = -0.2, -0.1, 0.1, 0.2$.
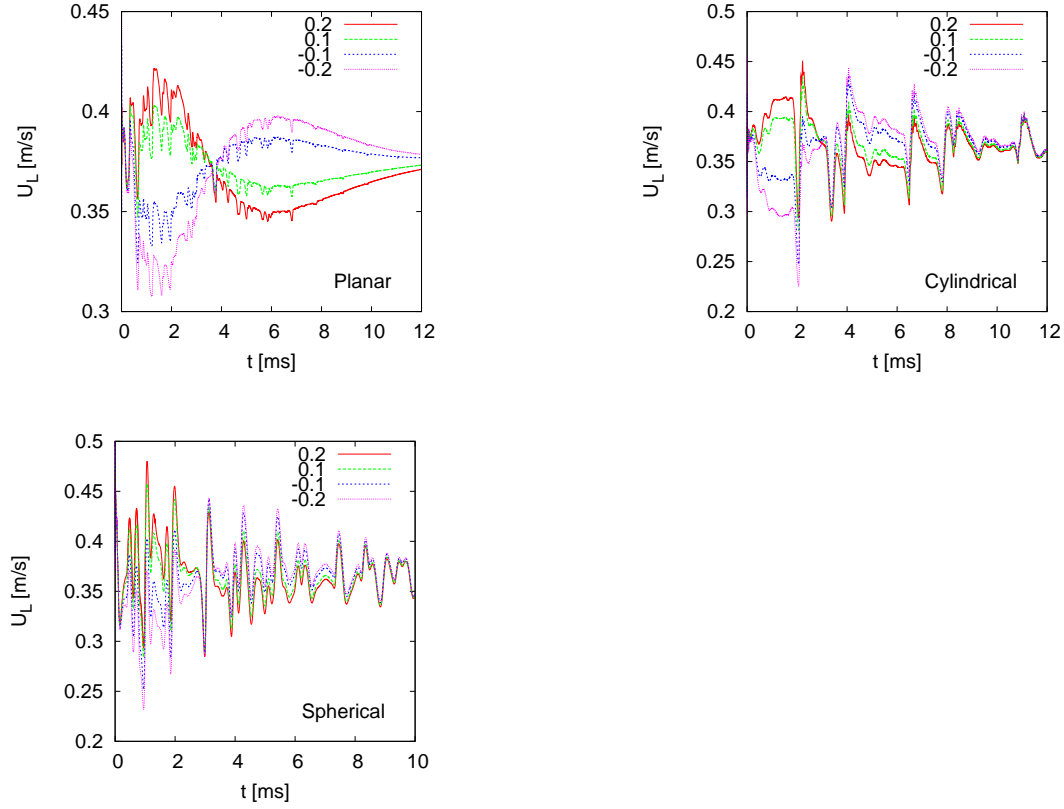

Figure 1: Laminar flame speed. Values of A_ϕ as indicated

Malik & Lindstedt [1] investigated stoichiometric H_2–air flames using a similar approach to that considered here. In contrast to CH_4–air flames, Hydrogen-ir flames have smaller thickness and chemical time scale. We can estimate the laminar flame thickness from $\delta_L \sim D_{th}/U_L$, where $D_{th} = \lambda/(\rho C_p)$ is the thermal diffusivity evaluated in the fresh gases, λ is the thermal conductivity and C_P is the heat capacity at constant pressure, and ρ is the density. From this a laminar flame time scale can be estimated, $t_L \sim \delta_L/U_L$. For the Hydrogen-air system at stoichiometry these was found to be $\delta_L \sim 0.03mm$ and $t_L \sim 0.02ms$; and for the methane-air system the estimates are $\delta_L \sim 0.08mm$ and $t_L \sim 0.2ms$.

We define a new quantity, see [1], the relaxation time τ_R as the time that the burning velocity U_L-curves in Fig. 1 first cross-over – this is a quantity that provides a measure of the time scale of unsteady processes in the system. Furthemore, a non-dimensional number which we may call the relaxtion number n_R can be obtained from τ_R by dividing it by the flame time scale t_L, viz

$$n_R \quad = \quad \frac{\tau_R}{t_L} \tag{3}$$

In [1] it was found that the relaxation times for outwardly propagating stoichiometric hydrogen-air flames in planar/cylindrical/spherical geometries were, respectively, 0.8 ms, 0.7 ms and 0.6 ms. As can be seen in Figure 1 above, the corresponding relaxation times for outwardly propagating CH_4–air flames were found to be much longer at 4.0 ms, 3.5 ms, 3.0 ms. The latter values are roughly a factor of 5

larger than for the hydrogen–air system. But when non–dimensionalised, the relaxation number for the methane–air systems $n_R \sim 20, 17, 15$ are *smaller* than for the corresponding three Hydrogen–air flame geometries, $n_R \sim 48, 42, 36$, by about a factor 2.5 when using this scaling. The large values of n_R for the Hydrogen-air flame is due to the exceptionally small time scale t_L which is about 1/10th of that for the methane-air flames.

The methane–air flames display long tails in Figure 1 after they first cross over, so long in the case of the planar flames that they have not returned to the mean value even after 12 ms. This is probably because the scalar diffusion velocity V_F (which we define in term of the flux of the fuel mass fraction $J_F = \rho Y_F V_F$) is greater than the laminar flame speed U_L and so the flame will reach the mean limit at $\phi = 1$ asymptotically at inifinity. The curved flames also display long tails, although they do attain to the mean value in a finite time indicating that positive stretch has enhanced the local flame speed such that $U_L > V_s$.

It may also be noted that in the planar flame, the pressure fluctuations have all but decayed out around 7 ms, but in the curved flames the fluctuations are surprisingly persistent even at 10 ms. This is important because it suggests that flame geometry may play an important role in sustaining pressure fluctuations. This mechanism warrants a separate investigation, but we may note that the focusing of pressure waves as they propagate inwards may contribute to this mechanism. As the flames are placed close to the centre at around $r \sim 10 - 20mm$ even small pressure fluctuations can build up to produce large amplitudes, which is manifested in Figure 1 as large spikes in U_L. The biggest spikes show a periodicity which is due the periodic reflection of acoustic waves at the curved boundaries. The gradual decay of the fluctuations due to the action of viscosity is particularly evident in the spherical flame.

Figure 2 shows the profiles of six selected species, H, OH, HO_2, CH, CO and CHO. There are obvious differences as compared to the corresponding profiles in the Hydrogen-air system; for example, the H–radical profile is broader. However, the OH–profile remains relatively broad and the HO_2–profile thin. The CH–profile is very thin. The general trend follows the observations of Lindstedt & Malik [1] and Malik [2] with respect to the relative thickness of the species profiles to the wavelength of the physical disturbances, even though the response of particular species may differ from system to system. The CH– profile is not affected by the pressure fluctuations and otherwise is only affected in peak amplitude which adjusts to the local equivalence ratio fluctuations. However, the OH–profile is disturbed across its whole length and in its peak amplitude. The CO–profile is broad compared to the acoustic length scale and is disturbed across its length. Formaldehyde, CH2O, is thin and appears undisturbed in its profile and even its peak amplitude appears to be marginally affected in comparison to the CH peak amplitudes which varies significantly. The HO_2 reaction zone is fairly thin and shows little change in its shape.

Interestingly, the H–profile is thicker in the methane-air flame than in H2-air flames [1] but shows surprisingly little disturbance. Clearly the thermochemistry is highly non-linear inside the flame kernel and the coupling of the pressure oscillations to the chermical kinetics and to the transport processes affect different species to varying extents.

By the ICDERS 2009 conference, the complete set of results pertaining to planar and curved flames subjected to stretch and inhomogeneous fuel distributions, particularly with relation to possible time-lag of the local rate of heat release, and Markstein length analysis, as well as a comparison to the hydrogen-air flames will be presented.

References

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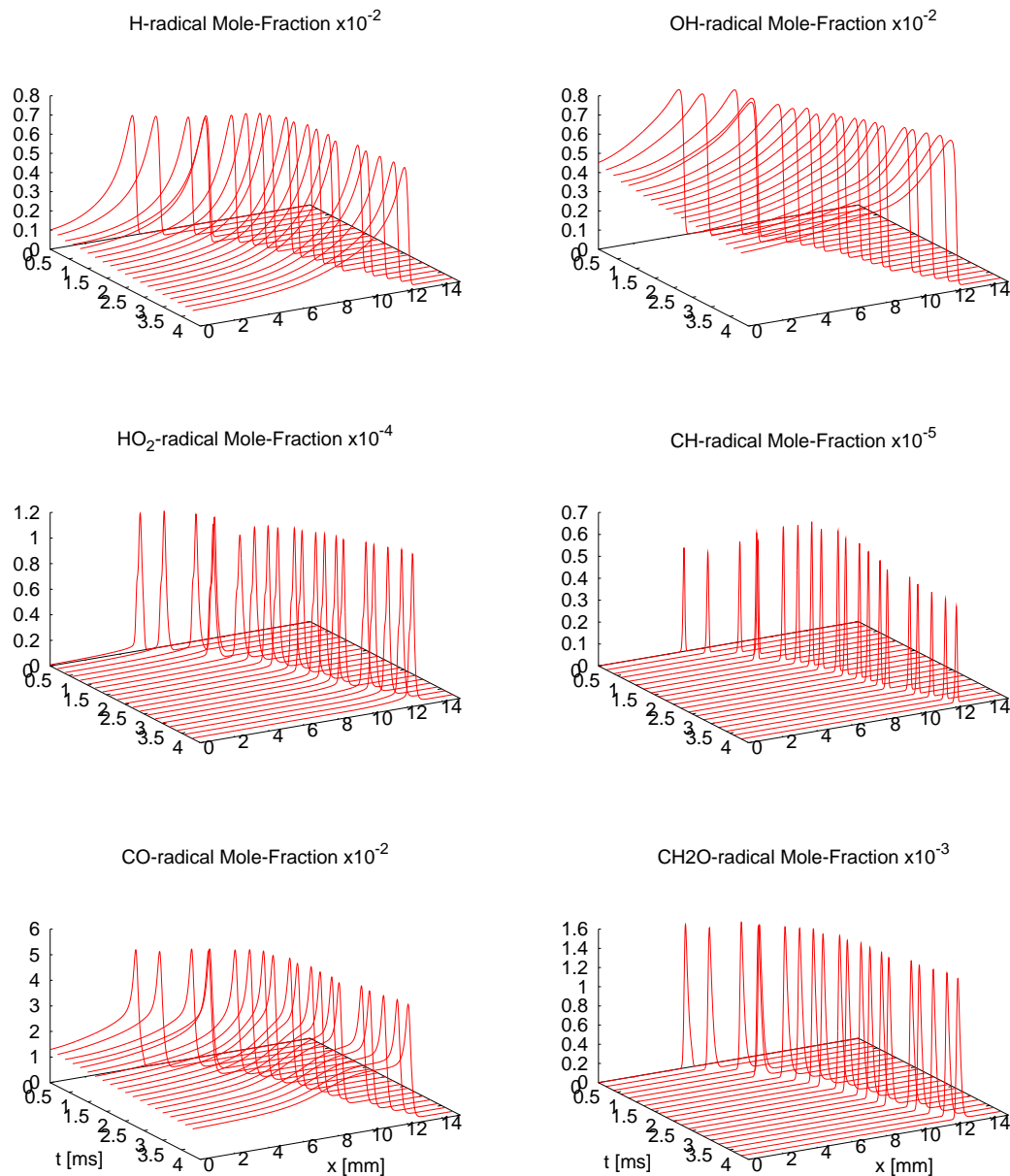
H-radical Mole-Fraction x10^{-2}

OH-radical Mole-Fraction x10^{-2}

HO$_2$-radical Mole-Fraction x10^{-4}

CH-radical Mole-Fraction x10^{-5}

CO-radical Mole-Fraction x10^{-2}

CH2O-radical Mole-Fraction x10^{-3}

Figure 2: Mole-fractions of indicated species against time and position. Planar flame.

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