The Response of Premixed Laminar Flames to Pressure and Equivalence Ratio Fluctuations

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1   Introduction

The study of transient propagating flames featuring detailed chemical kinetics is now possible due to improvements in computational hardware and solution algorithms. Early efforts featured the use of simple chemical systems, such as hydrogen, and parallel computing facilities (e.g. Lindstedt and Sakthitharan 1998 [1]). However, more complex fuels such as methane and propane were also considered (Lindstedt et al. 1998 [2]; Meyer (2001) [3]). The sensitivity of flames to parametric variations in properties such as the equivalence ratio (Marzouk et al. 2000 [4]; Sankaran and Im 2002 [5]), induced pressure fluctuations (Lindstedt and Malik 2001 [6]; Teerling et al. 2005 [7]) and harmonic velocity fluctuations (Lieuwen 2005 [8]) have also been explored. It has also been observed in past studies that flames feature "memory effects", which may result in extended flammability limits or a greater ability to resist strain (e.g. Christiansen and Law 2002 [9]). The response of a flame kernel to pressure fluctuations can lead to violent amplification of the heat release, while lean gas mixtures can be difficult to ignite and sustain, with the possible consequence of self-induced oscillations. For example, recent work on the control of combustion oscillations in a round duct with stratified premixed flows, has shown that forcing the flow at discrete frequencies reduced the rms of the oscillations by as much as a factor of four and peak to peak pressure variation, caused by the cycles of extinction and relight, by up to factor of ten (Luff et al. 2007 [10]). Interestingly, it was found that a range of forcing frequencies up to of the order 1000 Hz were effective. The impact of pressure fluctuations upon combustor stability has been highlighted in a number of studies (e.g. Candel 2002 [11]). Particular attention has been given to topological effects related to flame surface area generation in turbulent flows. As part of such studies, approaches that do not provide a direct coupling to the thermochemical flame structure (Schuller et al. 2002 [12]) or, alternatively, very simplified 1-step chemistry (e.g. Teerling et al. 2005 [7]) have been used. Such studies do show that instabilities are amplified when several spatial dimensions are considered. There is also direct evidence that the intrinsic thermochemical structure may lead to pulsating instabilities as shown by Christiansen and Law (2002) [9]. The research team of Vlachos (Gummalla and Vlachos 2000 [13]) has investigated the influence of the thermochemical structure of the flame on the occurrence of pulsating combustion. The current work explores the response of laminar flames subjected to both pressure and equivalence ratio fluctuations.

2   Aims

The aims of the current work is to clarify the impact of equivalence ratio fluctuations upon rates of heat release and to elucidate the underlying physics of fundamental thermoacoustic interactions at frequencies that may couple to the thermochemical structure of flames. Specifically, the coupling of equivalence ratio

variations with pressure oscillations is explored in the context of the impact upon the inner reaction zone structure of flames at certain frequencies. The work is performed in the absence of geometric complexities through a simplified direct simulation method featuring the propagation of transient flames in a fully compressible flow. In the current abstract, the simulation method is first outlined briefly, which is followed by results obtained from equivalence ratio variations in a propane-air system. The focus of the discussions is on the response of integral properties, such as the laminar burning velocity, as well as on the rate of radical production.

3   Method

Simulations have been performed using two calculation methods for fully compressible reacting flows. The first is a Lagrangian approach stemming form the work of Lindstedt and Sakthitharan (1998) [1] and Lindstedt et al. (1998) [2]. This method has been further developed for a planar (or cylindrical/spherically symmetric) geometry. The second calculation method (Lindstedt and Malik 2001 [6]) is Eulerian in which a Poisson equation for the pressure field was solved using a PISO-type method. The latter calculation method has the advantage that strain and curvature effects can be considered through outward and inward propagating flames while coupled to pressure oscillations. The solution method is second order accurate in space and time, and the chemistry is a C1-C3 subset of the C1-C6 chemical mechanism derived by Lindstedt and Skevis (1997) [14] and Lindstedt and Meyer (2002) [15]. The mechanism features 300 chemical reactions and 48 species. In both methods, the balance equations were discretised using central differencing in an implicit finite volume framework on a staggered grid; the species fields are solved simultaneously using a Newton-Raphson expansion which yields a block implicit tri-diagonal system and this is solved iteratively to convergence.

4   Results & Discussion

The case discussed here considers a one-dimensional spherically symmetric propane-air flame at atmospheric pressure. The flame is ignited at the centre of the sphere, using a 0.5 mm wide hot pocket, and propagates through a single equivalence ratio fluctuation as shown in Fig. 1. The shape of the initial fuel distribution is well preserved for a reasonably long time. Thus for the corresponding non-reacting case (no ignition) the peak fuel concentration has only declined by around 4% at a time of 9 ms. The computation shown here features dynamic local grid refinement with the actual flame structure resolved by a minimum of 100 computational cells and with the Courant number < 0.5. The resulting evolution of the temperature profile is shown in Fig. 2, where the lines are separated by 1 ms in time. Consideration of Fig. 3, which shows the evolution of the integral laminar burning velocity, highlights several interesting findings. Firstly, the flame accelerates rapidly at first and reaches a propagation velocity that is close to that of the corresponding steady state stoichiometric mixture. Secondly, the increase in the stoichiometry to the corresponding fuel rich limit value ($\phi \sim 1.6$) does not lead the flame to approach the corresponding steady state value. Rather, the dip is much more modest. By contrast, the lean part of the fluctuation causes the flame to approach the expected limiting value rather more rapidly. The corresponding rates of H radical production are shown in Fig. 4. It is evident that the rate of production adjusts quickly to changes in the local composition. By contrast, as shown in Fig. 5, the actual H concentrations are less affected. The total rate of radical production through the flame structure is shown in Fig. 6 for three points located around the first peak in the hydrogen radical concentration shown in Fig. 5. Further results have been obtained for methane-air flames and with variations in the width of the equivalence ratio oscillation.

Furthermore, in an effort to study the coupling between acoustic pressure oscillations and thermochemical oscillations and their impact on the thermochemical structure of the flame kernel, we are currently in the process of examining the sensitivity of hydrogen and hydrocarbon systems in the context of a parametric study covering a wide range of coupled equivalence ratio and pressure oscillations.
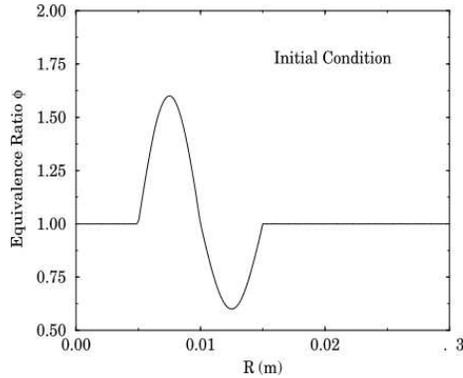
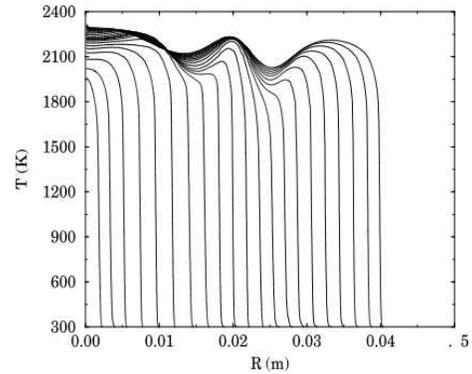**Figure 1**

Initial spatial distribution of fuel

Figure 2

Temperature evolution corresponding to Fig. 1.
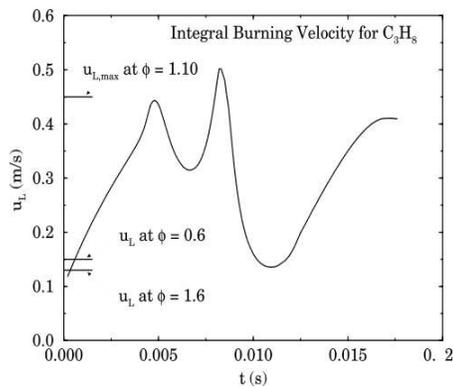The lines are separated by 1 ms in time

Figure 3

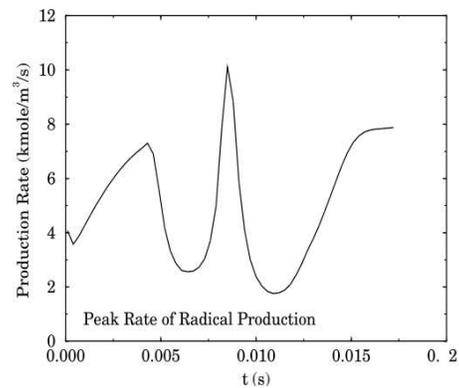Evolution of the integral burning

Figure 4

Peak radical production rate evolution.

Conditions have been selected to be of relevance to flame structures in practical geometries.

A stoichiometric hydrogen flame propagating in a planar geometry through a single equivalence ratio oscillation, characterised by a wavelength λ_ϕ and amplitude A_ϕ (thus, $1 - A_\phi \leq \phi \leq 1 + A_\phi$), is also subjected to acoustic pressure oscillations with a spectrum of frequencies E_p as shown in Fig. 7 where a few dominant frequencies between 4000 Hz and 50000 Hz are observed. The rms pressure fluctuation was $\sim 0.7\%$ of the mean (atmospheric) pressure.

Simulations were carried out for four cases: (1) $\lambda_\phi = 1\ mm$, $A_\phi = 0.1$, (2) $\lambda_\phi = 1\ mm$, $A_\phi = 0.2$, (3) $\lambda_\phi = 2\ mm$, $A_\phi = 0.1$, (4) $\lambda_\phi = 2\ mm$, $A_\phi = 0.2$. Figures 8 and 9 show, respectively, the integral laminar burning velocity and the rate of heat release. The effect of the equivalence ratio fluctuation is evident in the manner in which the burning velocity varies as a function of time; and the small scale fluctuations which are due to the pressure fluctuations can also be seen. It appears that at these low levels of pressure fluctuations the effect of equivalence ratio and pressure fluctuations can be decoupled and linearly added. This is particularly evident in the long time limit where all four cases show almost identical trends. However, it is important to note that amplification may also be possible depending on the frequency range studied and further investigations are required.

The amplitude of equivalence ratio fluctuations appears to diminish significantly even in these short
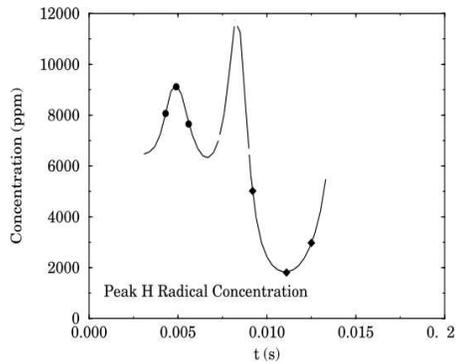
Figure 5
Temporal evolution of the peak H radical
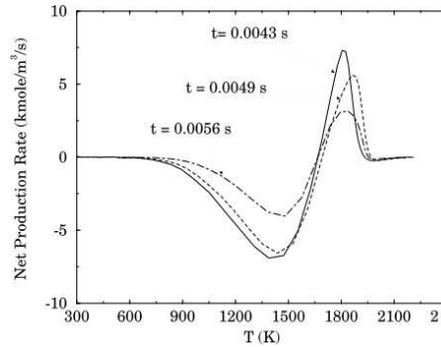concentration.

Figure 6
Radical production rates at the first
3 locations indicated in Fig. 5.

time and length scales, as seen in Fig. 10 which shows the fuel (H_2) mole fraction profiles at 0.5 ms
intervals for case (4). The rapid fall in the amplitude of the equivalence ratio fluctuation is probably
due to the small scale of the fluctuation λ_ϕ which produces very high initial gradients in ϕ which is
then rapidly diminished by diffusion. This is in contrast to the case described in Figs. 1-6 where the
fluctuation length scale is 10 times bigger (10 mm) and the amplitude diminished by just 4%.
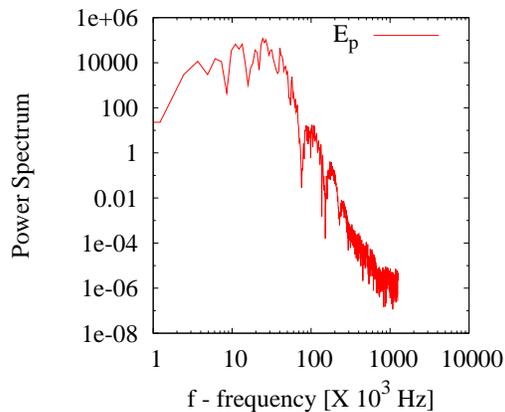

Figure 7
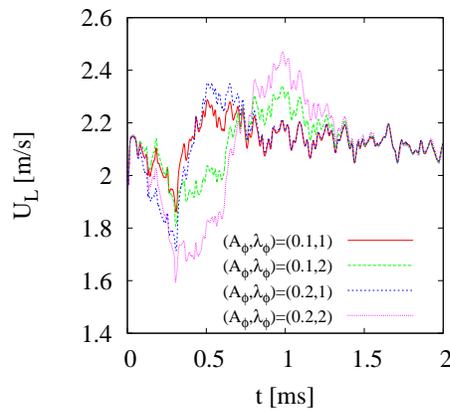Pressure fluctuation power spectrum

Figure 8
Integral burning velocity as a function of time

Of considerable interest is the thermochemical response of individual species profiles which our de-
tailed computational method allows us to examine. Figures 11 and 12 show at 0.5 ms intervals across
the domain, respectively, the mole-fraction profiles of OH and HO_2 radicals for case (4). The latter,
with a scale much smaller than 2 mm, is comparatively unaffected with only the peak values showing
significant oscillation, while the broader OH radical structure with a scale of several mm is clearly
perturbed across the entire width of the profile. It would appear that the response of different chemical
species depends, among other factors, on their spatial distribution with potential implications for the
overall flame structure through the reactive–diffusive coupling. For example, if $l_k/\lambda \sim 1$, where l_k is
the width of profile for species k and λ the wave length of the equivalence ratio or pressure oscillation,

then one may expect the species structure to show a response, and the effect on different species can be striking, as shown above. Further work is being carried to complete the parametric study, including more complex geometries such as spherical symmetric cases where the effects of local strain are present.
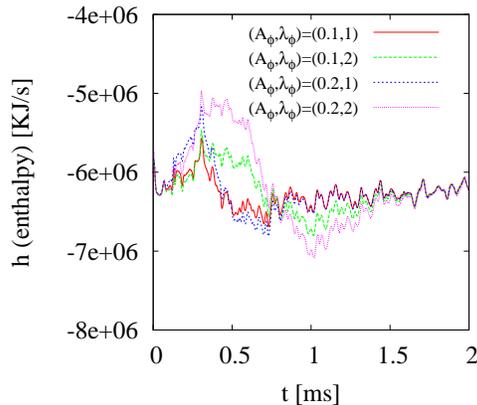

Figure 9
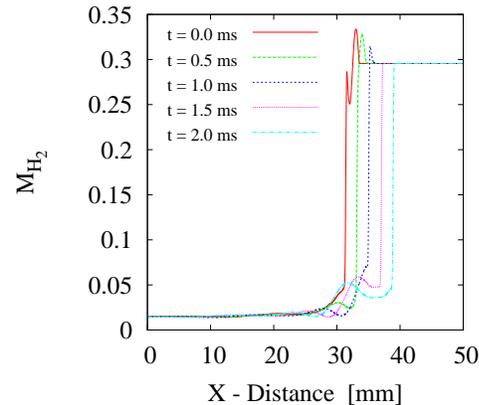Heat (enthalpy) release rate as a function of time

Figure 10
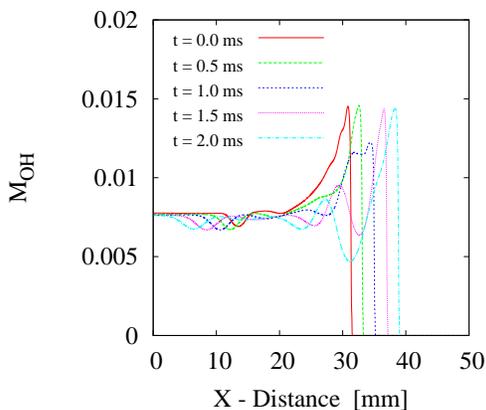Mole fraction of H_2 $(A_\phi = 0.2, \lambda_\phi = 2mm)$

Figure 11
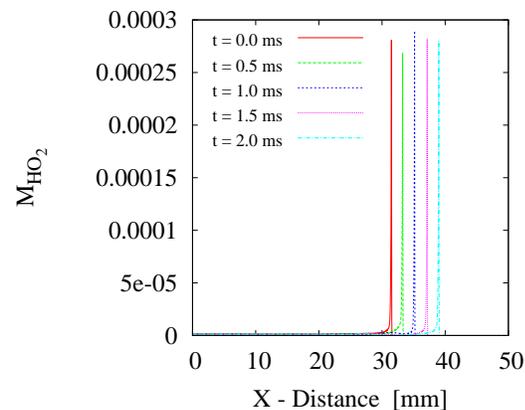Mole fraction of OH $(A_\phi = 0.2, \lambda_\phi = 2mm)$

Figure 12
Mole fraction of HO_2 $(A_\phi = 0.2, \lambda_\phi = 2mm)$

Acknowledgement

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