Premixed Flame Response to Disturbances in Pressure and Fuel Distributions

Nadeem A. Malik^{1,2} and R.P Lindstedt²

 ¹King Fahd University of Petroleum and Minerals, Department of Mathematics and Statistics, P.O. Box 5046, Dhahran 31261, Kingdom of Saudi Arabia
²Imperial College London, Mechanical Engineering Department, London SW7 2AZ, U.K.

1 Introduction

The impact of pressure and equivalence ratio oscillations on flames [1,2,3,4] is a critical issue in combustion with relevance to hazard analysis and propulsion devices such as gas turbines. The need to investigate such phenomena with realistic chemistry has never been greater as highlighted in a number of recent studies [5, 6, 7, 8]. The progress in numerical methods and computer technology now offers such a possibility and implicit solvers, in particular, have been receiving increased attention due to their greater stability [7, 8, 10]. Malik [7, 8] has developed an implicit combustion code TARDIS (Transient Advection Reaction Diffusion Implicit Simulations), featuring the coupling of compressible flow to comprehensive chemical mechanisms. The method can resolve all the convective and chemical length/time scales present in stiff chemically reacting systems. The current study investigates the response of premixed methane/air flames subjected to simultaneous pressure and equivalence ratio fluctuations for outwardly propagating planar, cylindrical and spherical flames in order to shed light on the underlying physics of thermoacoustic interactions and on the thermochemical flame structure under conditions of inhomogeneous fuel distribution and for different levels of stretch. We compare the obtained results with the hydrogen/air system reported in Malik and Lindstedt [7].

2 Method and Results

The current computational method has been described in [7, 8]; but briefly, it is an Eulerian method in which the fully coupled 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 solution algorithm is a fractional step finite volume scheme, second order accurate in temporal and spatial resolution. The applied chemical mechanisms are comprehensive and the C_1-C_2 chemistry features 30 species and 148 reactions with the hydrocarbon part as outlined by Lindstedt [11]. The hydrogen sub–system was obtained from Sun et al. [12] with the rate constant for the O + H₂ = OH + H reaction altered to the original CEC recommendation as outlined by Gkagkas and Lindstedt [9]. Thermodynamic data was computed using JANAF polynomials.

Transport properties are evaluated locally and are functions of temperature and composition; the specific Lewis numbers are non-unity which allows the effect of differential diffusion to be included. The current

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work therefore permits a direct comparison of two fuels, H_2 reported by Malik and Lindstedt [7] and CH₄, that feature not only very different chemistries, but also very different transport properties.

Random pressure fluctuations with frequencies in the range 200–1000 Hz were set up inside a domain size of length L = 400 mm. The fuel inhomogeneity was introduced as a sinusoidal oscillation cycle in the equivalence ratio just ahead of the flame front, viz $\phi(r) = 1.0 + A_{\phi} \sin(2\pi r/\lambda_{\phi})$, where λ_{ϕ} is the lengthscale of variation and A_{ϕ} is the initial amplitude. Four cases of moderate inhomogeneity $A_{\phi} \ll 1$ in each geometry were considered with $A_{\phi} = -0.2, -0.1, 0.1, 0.2$. Figure 1 shows a schematic of the simulation set up just as the flame is about to propagate into the equivalence ratio oscillation cycle.



Figure 1: Schematic of simulation set up

Figures 2 shows the burning velocity (fuel consumption rate) S_n against time as the flames move through the equivalence ratio oscillation in the three different geometries. The response of the flames to the fluctuating local conditions is evident in the variation of S_n and the qualitative trends are similar to those observed in the hydrogen/air system [7]; the burning velocity follows an underlying sinusoidal variation in the mean, decaying in amplitude due to the action of transport processes. However, the local fluctuations induced by the random pressure fluctuations are also evident.

The horizontal lines indicate the theoretical upper and lower bounds of the burning velocity for the corresponding homogeneous fuel distributions. The lower bound $S_L = 0.25$ m/s at $\phi = 0.8$ is not approached; but the upper bound at $\phi = 1.2$ appears to be reached, although this may be co-incidental because the burning velocity for this composition is similar to the stoichiometric value of $S_L = 0.37$ m/s with the maximum $S_L = 0.4$ m/s at $\phi = 1.15$. By contrast, the upper bound in the hydrogen/air flame was not approached [7].

We define a flame relaxation time τ_R as the time taken by the flame to return to its equilibrium value after the initial disturbance; from this a non-dimensional flame relaxation number, $n_R = \tau_R/t_L$ is defined where t_L is the flame time scale, which is indicative of a flame's stability to external disturbances; small values n_R indicates greater stability because the burning velocity returns swiftly to the underlying mean value. We observe that although τ_R in the methane/air flames is about 6 times longer than in hydrogen/air flames (when compared for similar geometries), the non-dimensional n_R are actually similar in both types of flames (4.2 Planar; 3.2 cylindrical; 2.8 spherical) indicating a similar level of stability. Note that n_R is a strong indicator of the effects of stretch; it increases as the curvature decreases from spherical to planar flames, as shown in Figure 2.

The chemistry-transport coupling was also found to differ in the respective pressure spectra. Malik and Lindstedt [7] found that the pressure frequency in H₂-air flames scaled like ω^{-2} ; but the CH₄-air flames



Figure 2: Computed flames speed S_n [m/s] against time [ms], from (a) Planar (b) Cylindrical (c) Spherical flames. Amplitudes of the initial sinusoidal equivalence ratio variations are 0.2 (red), 0.1 (green), -0.1 (blue), -0.2 (purple). Turqoise horizontal lines indicate the unstretched flame speed at the upper and lower bounds of the equivalence ratio osicalltion, i.e. at $\phi = 1.2$ and 0.8.

display a weaker response, ω^{-3} in the planar and cylindrical geometries, see Figures 3(a) and 3(b). For the spherical geometry the spectral response was even weaker as shown in Figure 3(c).



Figure 3: Log-log plots of the pressure-frequency spectrum: (a) Planar (b) Cylindrical and (c) Spherical flames.

The profiles of individual chemical species inside the flame structure were found to show markedly different responses to the disturbances – chemical species with a reaction layer length scale l_k less than the length scale of physical disturbance λ are too thin for the shape of their profiles to be altered, although their peak values are changed in response to the local conditions. Species with broad reaction zones, on the other hand, are significantly disturbed, except for the major reactants and products which show little response. This re-enforces the idea introduced in [7] that it may be more appropriate to analyse flames in terms of a *spectrum* of species length scales (l_k) rather than just a single global scale.

Lindstedt and Malik [7] reported that the mole fractions of H and O radicals were approximately anticorrelated in hydrogen flames with the trend reduced under the influence of strain. It was suggested that the result may partly be influenced by the main chain branching reaction (H + $O_2 = O + OH$). It was also shown that the heat release was correlated with the H radical. The current system is chemically more complex and provides an opportunity to assess the corresponding impact on the flame structure. As shown in Figures 4a and 4b, where results from a planar CH_4 flame have been chosen to illustrate the effect, a similar anticorrelation is observed. As also shown, the methyl radical appearance is correlated with the H radical increase and the removal of the O atom. The dominant reaction paths for CH_4 removal pass via H and O attack with both channels leading to the CH_3 radical.



Figure 4: Species mole fractions X_i versus distance r [mm] from planar flame: (a) H radical (b) O radical (c) CH₃ radical.

3 Conclusions

The impact of pressure oscillations in the range 200 - 1000 Hz on CH₄/air flames in different geometries was examined and compared to results from corresponding calculations of H₂/air flames reported by Malik and Lindstedt [7]. The spectral response was found to be weaker, $E(\omega) \sim \omega^{-3}$ (or less), than for the hydrogen flames, where $E(\omega) \sim \omega^{-2}$, which reflects the weaker chemistry-transport coupling in methane flames. However, the non-dimensional flame relaxation number $(n_R - \text{defined as the time that})$ the flame speed takes to return to its mean value after disturbance, divided by the flame time t_L) was found to be similar in both types of flame, which indicates a similar stability to pressure disturbances. In absolute terms, the flame relaxation time is about 6 times longer than for the corresponding hydrogen flames. Other qualitative features are similar to those observed for hydrogen flames. This re-enforces the idea introduced [7] that it may be more appropriate to analyse flames in terms of a spectrum of species length scales (l_k) rather than just a single global scale. The methyl radical appearance is correlated with the H radical increase and the removal of the O atom - probably due to the dominant reaction paths for CH_4 removal, which pass via H and O attack, with both channels leading to the CH_3 radical. The anti-correlation between H and O radicals observed in hydrogen flames is reproduced for the current methane flames. This study has been facilitated by the new implicit method TARDIS [7,8] which couples the compressible flow field to the comprehensive chemistry and detailed transport properties. This allows realistic flames with stiff chemistry to be simulated under strongly unsteady and inhomogeneous conditions and subject to pressure disturbances that interact with the flame kernel.

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