

Thermochemical scales and structure in stretched laminar flames: a numerical study using realistic chemistry

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1 Introduction

A question of great importance in combustion theory is how to characterise the flame length and time scales – it is surprising that to date there is no universally accepted theory. This is relevant not only to laminar flame theory, but also to combustion under turbulent conditions because turbulence itself is characterised by a continuous range of length and time scales.

One of the most important concepts in combustion theory is flame stretch, $\kappa = (dA(t)/dt)/A(t)$, which is the relative rate of change of an element of surface area $A(t)$ on the flame surface.

Stretch quantifies the effect of local heat release of a propagating flame on variations in the surface area along the flame front and the associated local flame curvature; as such stretch is sensitive to the local strain and to the flame geometry, which in turn affects physical quantities like the flame speed S_n . For axi-symmetric and spherically symmetric flames stretch scales like, $|\kappa| \sim 1/r_u$ where r_u is the flame radius; see [1] for details.

In this study we explore the thermochemical structure of stretched laminar flames through simulations of eight configurations of premixed flames at atmospheric pressure and at stoichiometric mixture levels: hydrogen/air and methane/air flames propagating *outwardly* and *inwardly* in axi-symmetric and spherical geometries. The aim is to examine the sensitivity of the flame structure to stretch and to explore consistent methods of characterising the flame thickness and the associated time scales.

The method adopted is numerical, using the implicit code TARDIS (Transient Advection Reaction Diffusion Implicit Simulations) [1–3]. TARDIS *couples the compressible flow to the comprehensive chemistry and detailed multicomponent transport properties*, and as such it resolves all the time and spacial scales in the stiff thermochemical systems examined here – a step towards realistic combustion simulations. TARDIS is a new method with complete coupling between the flow, chemistry and transport properties – few previous methods possess this capability. This gives us an opportunity to explore the internal structure of flames in unprecedented detail.

Comprehensive chemical schemes for H₂/air [7] and for CH₄/air [8] are used to model the chemistry.

2 Flame Length and Time Scales

A number of different definitions of flame thickness is current in the literature: the ‘momentum’ thickness $\delta_L^\nu \sim \nu/s_L$, where ν is the kinematic viscosity, and the time scale is then $t_L^\nu \sim \delta_L/s_L$; a thermal thickness as $\delta_L^D \sim D^{th}/s_L$ where D^{th} is the thermal diffusivity, and hence $t_L^D \sim \delta_L^D/s_L$; the distance between certain isotherms of flame temperature δ_L^p and the associated time scale is t_L^p ; however, the choice of isotherm is arbitrary.

The profiles of the fuel consumption rate \dot{R}_F also provides an estimate for flame thickness, δ_L^R – this is the physical extent of the reaction layer.

Göttgens et al. [4] derived an analytic approximation for the flame thickness for a number of lean hydrocarbon and hydrogen flames.

We also have a range chemical time scales t_c associate with the reactive chemical species in the system. But for most commonly occurring flames the smallest time scale is around $t_c \sim 10^{-6}$ s, see [5].

Malik and Lindstedt [3] found that $\delta_L^R \approx 0.5$ mm for both H2/air and CH4/air flames – they possess approximately the same flame thickness using this definition.

Furthermore, from their study of flame-pressure interactions, Malik and Lindstedt [2,3] have argued that the idea of a single flame thickness maybe an over simplification, and suggested that a range of flame length and time scales may be a better way of characterising the flame kernel. Khateeb et al [6] hold a similar view.

3 The thermochemical flame structure

Figure 1 shows the flame structure, in terms of the mole fractions of chemical species, in inwardly propagating CH4/air flame at different times, when $r_u \sim 10$ mm (left), and when $r_u \sim 2$ mm (right). Different levels of stretch correspond to different locations of the flame at radius r_u , because the stretch scales with the curvature. The difference in curvature is about a factor of 5, nearly an order of magnitude. (Note that the stretch is negative in inwardly propagating flames.)

Two features are noteworthy here. First, different species possess different thicknesses, from a fraction of a millimetre to several millimetres. This echos the findings of Malik and Lindstedt (2010,2012) and Khateeb et al (2011).

Second, the flame struture in terms of the mole-fraction remains practically unchanged even though the level of stretch changes by an order of magnitude.

Expanding CH4/air flame show similar structure (execpt reflected from left to right). H2/air flame structures based upon mole fractions display qualitatively similar insensitivity to stretch.

Could there be a more sensitive indicator of local conditions than mole fraction profiles?

Figure 2 shows the production rates, \dot{R}_k [$Kg/m^3/s$], of some of chemical species in the inward CH4/air system at two different locations (times). Fig2(a) shows the \dot{R}_k profiles for, H2, O2, H2O, H, O, OH, HO2 and H2O2; Fig2(b) shows the \dot{R}_k profiles of some other selected speies. For direct comparison the profiles are shown close together on false abscissa which acts simply as a local scale. The solid profiles are located at $r \sim 20$ mm, and the dashed profiles are located at $r \sim 4$ mm.

There are clearly observable differeneeces in the peak values of most of the species reaction rates R_k , although the shape of the profiles remain almost unchanged. This is important because if R_k is more sensitive to variations in local curavture than species mole-fraction struture, it indicates suggests that reaction rates are more appropriate for examining the internal structure of flames.

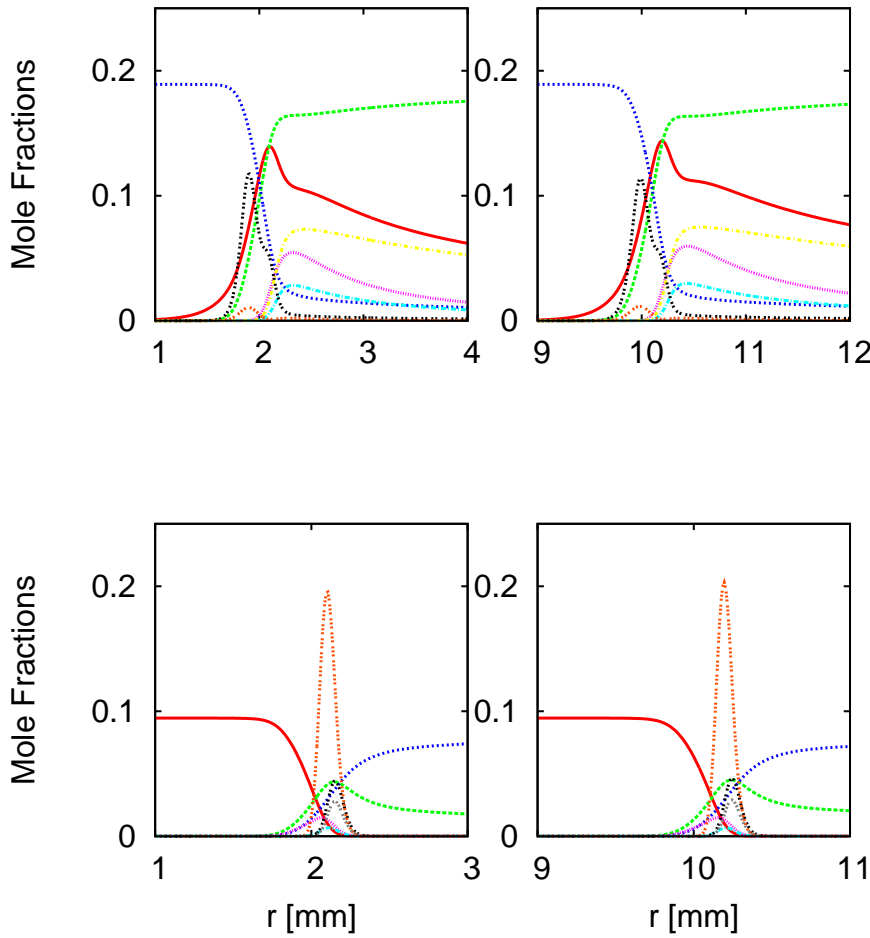


Figure 1: Mole fractions of chemical species, from *inwardly* propagating CH₄/air flame, against the radius at two different locations. **Top:** H₂ (red), H₂O (green), O₂ (blue), H (purple), O (turquoise), OH (yellow), HO₂ (black), H₂O₂ (brown). **Bottom:** CH₄ (red), CO (green), CO₂ (blue), CH₂ (purple), CH₂O (turquoise), C₂H₂ (black), C₂H₄ (brown), C₂HO (grey)

3 A classification of the reaction layer

A close examination of the profiles of individual species reaction rates in Figure 2 (and similar results for other flames that are not shown here) show patterns which are characterised by the number of zero-crossings, N_0 , along the abscissa. This is related to the number of turning-points N_p that appear in the profile, $N_p = N_0 - 1$. The results here show that, $1 \leq N_p \leq 5$ and $2 \leq N_0 \leq 6$. Figure 3, summarises the findings as a sketch. (Note, we count zeros at infinity as a zero-crossing in this definition.)

The major reactants and products (H₂, O₂, CH₄, H₂O, CO₂) display a single peak $N_p = 1$, but other species have $N_p > 1$. This is because minor species are created and destroyed, sometimes more than once, across the flame brush which appear as positive and negative reaction rates which produces the multiple-peak structure for the different species.

It was observed that the number of turning-points N_p is *different for the same species in different flame types*, reflecting the different kinetic-transport balance in the different flames.

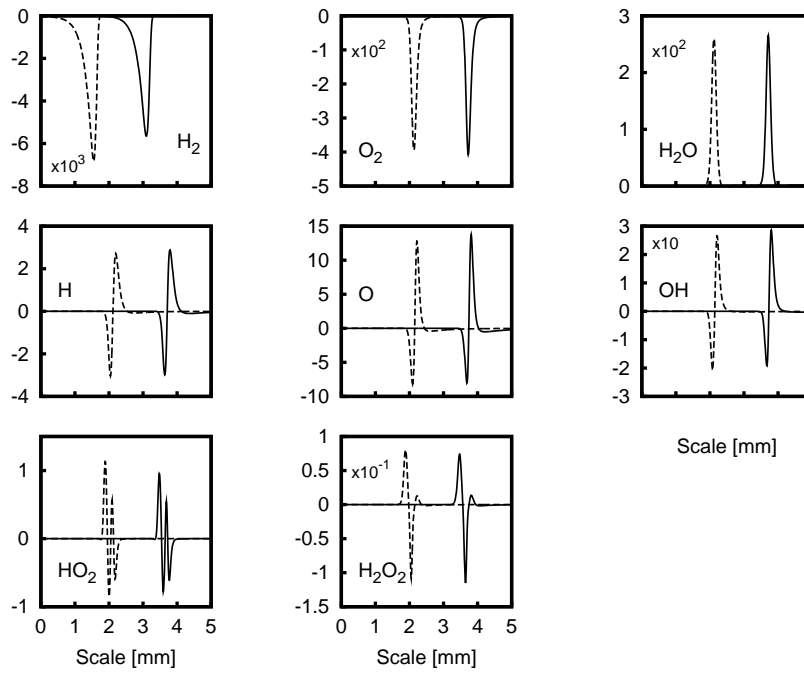


Figure 2: (a) Rates of production [$kg/m^3/s$] of selected chemical species against length scale [mm] from CH_4/air flame. Solid lines, at $r_u \sim 20mm$; dashed lines, at $r_u \sim 4mm$.

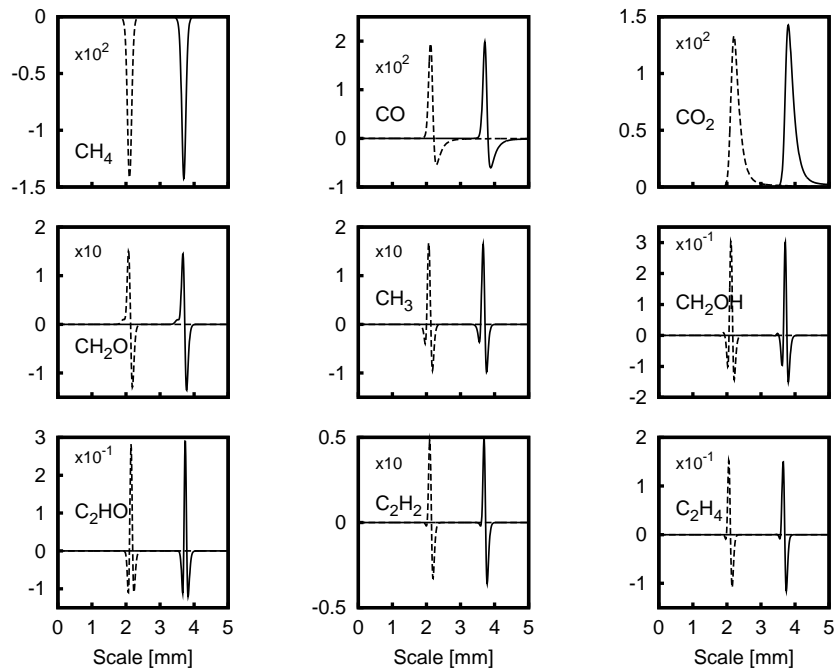


Figure 2: (b) Rates of production [$kg/m^3/s$] of other selected chemical species against length scale [mm] from CH_4/air flame. Solid lines, at $r_u \sim 20mm$; dashed lines, at $r_u \sim 4mm$.

There is a spectrum of length scales L_k^R in each flame – a factor of 2 in the methane flame and a factor of 4 in the hydrogen flame.

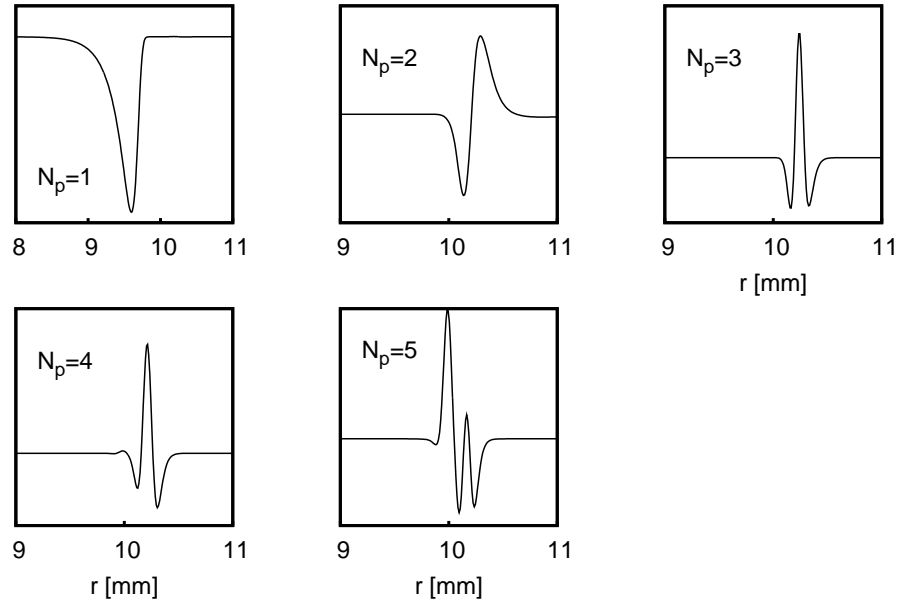


Figure 3: The five characteristic production rate profiles of chemical species, with N_p peaks as indicated. (Taken from methane/air spherical flames, clockwise from top left: H_2 , H , C_2HO , HO_2 , CH .)

4 Discussion

In this study we have investigated the thermochemical structure of premixed laminar flames, with the aim of elucidating characteristics of the inner reaction layer that are sensitive to the local conditions. This was done through comparing the response of flame structures in inwardly and outwardly propagating, hydrogen/air and methane/air flames in cylindrical and spherical geometries, at stoichiometric mixture levels and at atmospheric pressure in simulations using TARDIS [1–3].

Our results show that the flame structure in terms of *mole fractions* is insensitive to levels of stretch (differing by about an order of magnitude) even though the flame speed S_n displays observable changes under the same conditions, as shown in [1].

But the corresponding profiles of species *reaction rates* \dot{R}_k display observable changes under the same conditions, suggesting that reaction rates are a better indicator of local conditions than mole fraction profiles.

A novel classification of the inner reaction layer in terms of patterns observed in the reaction rate profiles \dot{R}_k is proposed: species profiles are characterised by the number of turning points N_p . This is related to the number N_0 of zero-crossings that the profile makes with the abscissa, $N_0 = N_p + 1$. In the flames considered, it was found that $1 \leq N_p \leq 5$. The main reactants and products display $N_p = 1$ peak; but other species have $N_p > 1$ because they are created and destroyed across the flame brush, sometimes more than once.

The spectrum of species thickness $\{L_k^R\}$ obtained from the rate profiles display a range of scales, strengthening Malik and Lindstedt's proposal that a range of length and times scales may be a more appropriate way to characterise flames than just a single global length and time scale.

The importance of this classification lies in its potential to characterise flame length and time scales and flame structure in a consistent manner, which could lead to new modeling strategies in the future. Although it is early days, it is possible to at least pose some modelling strategies that could incorporate the ideas that have emerged from this study. For example, it may be possible to divide the flame kernel into a multi-layered structure, where each sub-layer of thickness $\delta_f \approx L_f/N_P$ is characterised by the mean values of thermo-chemical quantities (species mass fractions, temperature, etc) within that sub-layer. L_f is the largest length scale in the flame kernel based upon reaction rates.

Further work is being carried out on a parametric study of the flame structure with respect to variations in equivalence ratio and pressure. At a later stage, work on different reaction mechanisms will be considered.

Acknowledgment

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