A Numerical Study of the Markstein Hypothesis in Finite Thickness Flames with Realistic Chemistry

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1 Introduction

Markstein's hypothesis for the burning velocity of stretched laminar flames characterizes 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. However the general validity of Markstein.s theory is still debated in the combustion community; of special interest is whether this hypothesis is valid under conditions of realistic chemistry in finite thickness flames.

The need to describe reacting systems with realistic chemistry has been recognised in a number of recent studies, [1, 2, 3]. One of the main drivers behind this trend relates to the energy and environmental sectors; restrictions on emissions of greenhouse gases, NOX, soot and other hazaradous substances to lower and lower levels places greater demands on the development of new fuels and on the optimisation of devices such as automotive engines and gas turbines. This in turn places greater demands on the accuracy of predictive simulations which must now include realistic chemistry.

A critical issue, therefore, in the computational study of combustion and reacting flow systems is the capability of coupling of the unsteady compressible flow to the detailed chemistry and transport properties. The recent progress in numerical software and in computer technology now offers the possibility to meet these demands, and implicit methods in particular have been receiving some attention due to their greater stability, although at the cost of large memory requirements [3, 4]. In [3] an implicit combustion code TARDIS (Transient Advection Reaction Diffusion Implicit Simulations) was developed which features the coupling of the fully compressible flow to the comprehensive chemical mechanisms. The method can resolve all the convective and chemical length and time scales present in stiff chemically reacting systems.

In this study, TARDIS is used to investigate the Markstein hypothesis in premixed hydrogen/air and methane/air flames at atmospheric pressure. The flame stretch rate κ is the relative rate of change of an infinitesimal surface area $A(t)$ surrounding a point on the surface of a flame,

$$\kappa = \frac{1}{A}\frac{dA}{dt} \tag{1}$$

from which the non-dimensional Karlovich number Ka is defined,

$$Ka = \kappa t_c \tag{2}$$

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where $t_c \sim \delta_L/S_L$ is the chemical time scale, δ_L is the flame thickness (often taken to be $\delta_L \sim \nu/S_L$ where ν is the kinematic viscosity, and S_L is the unstretched laminar flame speed).

It is widely believed [5, 6, 7, 8, 9, 10, 11] that in the limit of thin flames and weak stretch the difference between the stretched and unstretched flame speed is given asymptotically by a linear expansion in parameters that affect the flame, such as the local strain rate, curvature and pressure, each of which is deemed to induce its own component of stretch with an associated *Markstein length scale (L)* as the constant of proportionality, viz

$$S_L - S_n \approx L_s\kappa_s + L_c\kappa_c + L_p\kappa_c + ... + O(\epsilon^2 S_L) \tag{3}$$

where ϵ is a small parameter, the ratio of the flame thickness to the convective length scale. The Markstein lengths yield Markstein numbers when non-dimensionalised by the flame scale, $Ma_n = L/\delta_L$.

In cylindrically and spherically symmetric laminar flames, only the strain and curvature contribite to the stretch, and both produce terms that take a similar form as functions of the flame radius, which is at the location of the flame front r_u. For the strain component,

$$\kappa_s = \gamma\frac{u_g}{r_u} \tag{4}$$

and for curvature (flame geometry) component,

$$\kappa_c = \gamma n_r\frac{S_n}{r_u} \tag{5}$$

where $\gamma = 1$ for cylindrical flames, and $\gamma = 2$ for spherical flames. u_g is the unburned gas velocity ahead of the flame, r_u is the corresponding radius, n_r is the unit normal to the flame surface pointing towards the fresh gases. For outwardly propagating flames, $n_r = +1$ and $u_g \neq 0$ and so both components of stretch, due to strain and curvature, affect the flame speed. For inwardly propagating flames, we have $n_r = -1$ and $u_g = 0$ and only the component of stretch due to the curvature is present which allows the effects of curvature to be studied in isolation.

The velocity deficit is then linearly proportional to the curvature (inverse of the flame radius) [12]; for expanding flames we have

$$S_L - S_n = L_s\gamma\frac{u_g}{r_u} + L_c\gamma\frac{S_n}{r_u} \tag{6}$$

while for inwardly propagating flames,

$$S_L - S_n = -L_c\gamma\frac{S_n}{r_u} \tag{7}$$

The Markstein concept is important as it provides a simple expression for the flame speed for small stretch rates, and has been used in models for flame propagation. However, it continues to be the subject of debate. Lipatnikov [13,14] believes the concept to be unsafe. Lipatnikov and also Lindstedt et al. [15] have pointed out that Markstien numbers are strongly dependent on the various definitions used and on the isotherm chosen on which it is defined. Further doubts have been raised in [3].

2 Numerical Method and Results

TARDIS has been described in [3]; 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

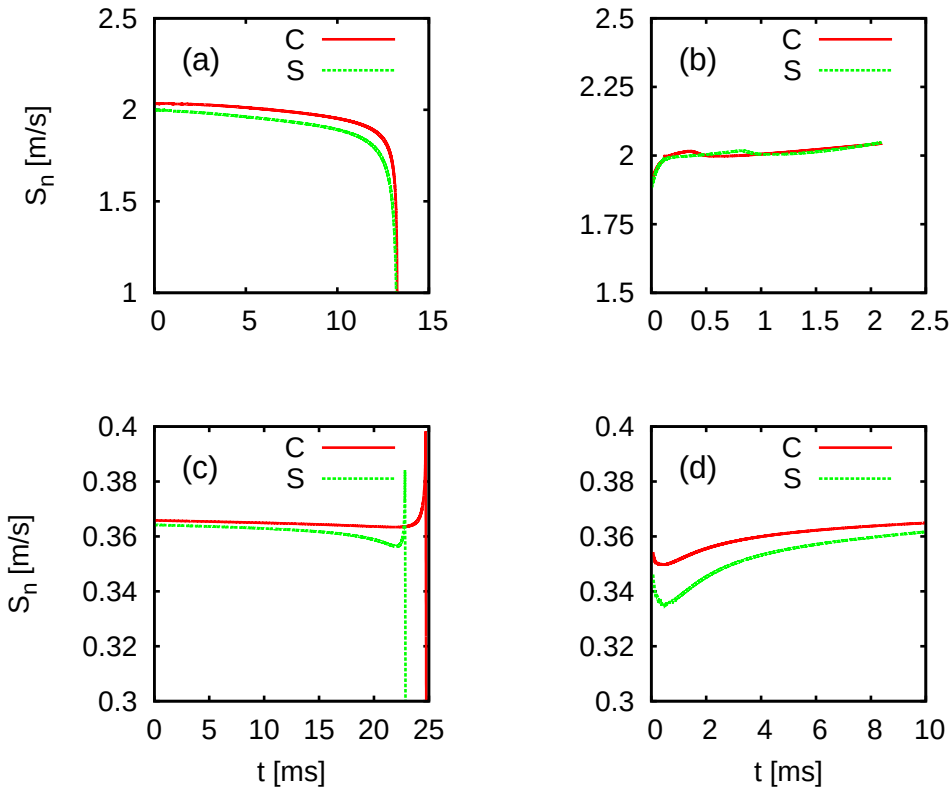

Figure 1: The burning velocity S_n [m/s] against time t [ms]. H2/air: (a) inward, (b) outward. CH4/air: (c) inward, (d) outward. C(red) – cylindrical flame; S(green) – spherical flame.

ideal gas, are solved in an implicit framework on a staggered grid arrangement. Transmissive boundary conditions were imposed on the gas velocity at the open (outer) boundary, and $u = 0$ at $r = 0$. The solution algorithm is a fractional step finite volume scheme, second order accurate in time and spatial resolution.

In this study, the chemistries are detailed systems of elementary reactions, featuring a 9 species and 30 reactions mechanism for the hydrogen/air (with the rate constant for the O+H2=OH+H reaction altered to the original CEC recommendation [16, 17, 18]; and a 30 species C1-C2 (each including up to two carbon atoms) and 148 reactions mechanism for the methane/air flames [19]. Thermodynamic data were computed using JANAF polynomials.

Viscosities and binary diffusivities were evaluated using the theory of Chapman & Enskog; thermal conductivities from the theory of Mason & Monchick. Mixture properties are evaluated from Wilkes formula, (see [3] for these references). Thus, all transport properties are evaluated locally and are functions of the temperature, which allows the system to be strongly inhomogeneous. The specific Lewis numbers are non-unity $Le_k \neq 1$ and functions of the local temperature; the Sorret thermal-diffusion for light-species (H and H2) are also included.

TARDIS has been validated by computing the laminar flame speed S_L directly from planar flame simulations without any further adjustments in the parameters. This is a critical test because TARDIS is a direct method and as such no adjustment of any parameters, other than the models for the transport properties and the chemistries, can be allowed. The flame speeds for H2/air and CH4/air for the stoichimetric conditions and atmospheric pressure under which the simulations were carried out were found

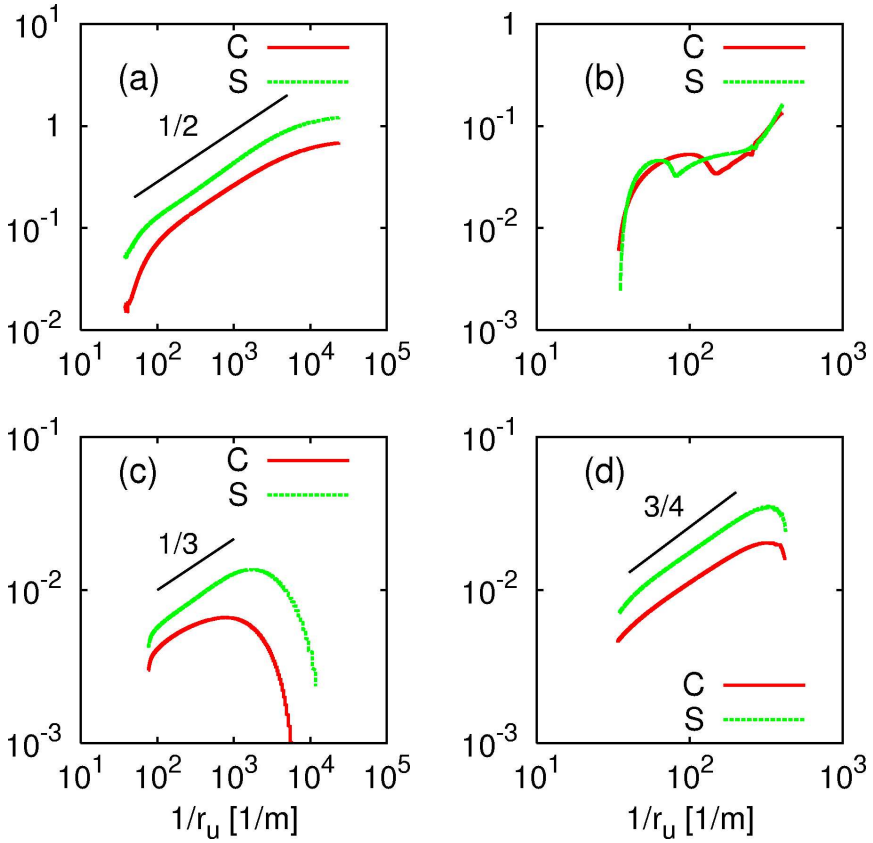

Figure 2: The velocity deficit $(S_n - S_L)$ [m/s] against $1/r_u$ [/m]. The ordering and labeling in the plots is the same as in Figure 1.

to be in good agreement with experimentally dertemined values to within experimental error; for H2/air we obtained $S_L \approx 2m/s$, and for CH4/air we obtained $S_L \approx 0.37m/s$.

The velocity deficit subject to stretch (curvature and strain) was investigated in a series of simulations of cylindrically and spherically symmetric flames. Eight cases of inwardly and outwardly propagating laminar stoichiometric H2/air and CH4/air flames at atmospheric pressure were considered. We define the flame speed (burning velocity) as the rate of consumption of the fuel integrated across the flame,

$$S_n = \frac{1}{\rho_u(Y_F^u - Y_F^b)} \int_{-\infty}^{+\infty} \dot{R}_F M_F dr \tag{8}$$

where F is the fuel ($H2$ or $CH4$), M_F is the molecular weight of the fuel and ρ_u is the density of the unburnt gases. Y_F^u is the unburned fuel mass fraction and Y_F^b is the burned fuel mass fraction (which is close to zero for stoichiometric and lean mixtures).

Figure 1 shows the burning velocity S_n against time, obtained from the simulations for the eight flame configurations considered: (a) inwardly propagating H2/air, (b) outwardly propagating H2/air, (c) inwardly propagating CH4/air, (d) outwardly propagating CH4/air. In each plot, the results from cylindrical (C) and spherical (S) flames are shown as indicated. (The simulations take a while to attain to the correct physical solution, this is especially noticeable in the outwardly propagating flames where initial numerical transients are observed in the first 0.2ms.)

The asymptotic stretched burning velocity approaches the unstretched laminar flame speed for large radius, $S_n \rightarrow S_L$ as $r_u \rightarrow \infty$, Figure 1(a) and 1(c).

The inwardly propagating methane/air flames show a sharp increase in the burning velocity just before total consumption of the fuel at the centre of the flame, Figure 1(c). This is possibly due to the build up of heat ahead of the flame which cannot diffuse away from the centre. The H2/air flame shows no such behaviour, Figure 1(a) – possibly because the thermal-diffusion of the light species may assist the transport of the heat generated away from the centre.

The log-log plots of the velocity deficit $S_n - S_L$ against $1/r_u$, are shown in Figure 2, (r_u is the location of flame front defined at the T = 305K isotherm) for the flames considered; non-unity fractional power laws in the curvature are observed, $S_n - S_L \sim (1/r_u)^p$ with $0 < p < 1$; the power p depends on the flame type and the mode of propagation. The black lines with fractional numbers indicate slopes for comparison on each plot.

The inwardly propagating CH4/air flames is close to $p = 1/3$; the outwardly propagating CH4/air flames is close to $p = 3/4$. The inwardly propagating H2/air flame is close to $p = 1/2$. Cylindrical and spherical geometries follow the same power law in each case, although cylindrical flame velocity deficit is consistently slightly greater than the spherical flame velocity deficit.

The expanding hydrogen/air flames in Figure 2(b) show anomalous behavior which is quite different altogether from a power law. This may be due to the fact H2/air contains the highest fraction of light species H and $H2$ which correspondingly will show the the greatest effect of the non-Fickian thermal-diffusion component which is proportional to the temperature gradient. On the other hand, the imploding H2/air flame in Figure 2(d) does display a power law behaviour, indicating that negative/positive curvature and the presence/absence of strain are also important factors in this complex process.

2 Discussion

TARDIS provides a powerful new numerical method which allows flames and reacting systems to be simulated in a realistic way with the compressible velocity field coupled to the detailed chemistry. Real flames have finite thickness and are subject to local variations in transport properties, and to differential diffusion and non-unity Lewis numbers within the framework of a comprehensive reaction sets. All of these effects are inlcuded in TARDIS, and the inclusion of detailed transport properties and comprehensive chemistry means that the results obtained from TARDIS can be asumed to represent physically real systems.

In this study, we have found that finite thickness H2/air and CH4/air flames at stoichiometry and atmospheric pressure do not follow the Markstein linear hypothesis for asymptotically thin flames. Rather, in the majority of cases fractional power laws in the velocity deficit of the form $S_n - S_L \sim (1/r_u)^p$ are observed with $0 < p < 1$; the power p depends on the flame type (H2/CH4) and mode of propogation (inward/outward). However, the power laws are the same in cylindrical and spherical geometries.

An exception is expanding H2/air flames which shows anomalous non-power law behaviour; this may be related to the Sorret thermal-diffusion component of diffusion which is strongest in H2/air flames. However, the absence of strain and presence of negative curvature in the inward H2/air flames appears to recover a power law behaviour, so the situation is much more complex than is apparent.

Current ongoing work has extended the study to explore other parameter ranges and conditions.

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