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Evaluation of models for flame stretch due to curvature in the thin reaction zones regime

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Abstract

Direct numerical simulation (DNS) was used to study modelling assumptions for the curvature-propagation component of flame stretch in the thin reaction zones regime of turbulent premixed combustion, a regime in which small eddies can penetrate the preheat zone but not the thinner fuel breakdown zone. Simulations of lean hydrogen–air and methane–air flames were conducted, and statistics of flame stretch due to curvature, henceforth referred to simply as stretch, were extracted from a species mass fraction iso-surface taken to represent the flame. The study focussed on investigating the modelling assumptions of Peters [J. Fluid Mech. 384 (1999) 107]. It was found that the mean stretch is dominated by stretch due to correlations of flame speed with curvature, and specifically the effects of tangential diffusion. The modelling suggestions of Peters were found to provide an improvement over the assumptions of a constant flame speed or a flame speed governed by the linear relationship with stretch at small and steady stretch. However for the conditions considered here, diffusive-thermal effects remain well into the thin reaction zones regime, and the suggestions of Peters generally over-predict the mean compressive stretch. An effective diffusivity for flame stretch was suggested and evaluated for the methane simulations. It was found that the effective diffusivity was comparable to the mass diffusivity for flames with a high ratio of flame time to eddy turnover time. The length scales contributing to stretch were investigated, and it was found that while most flame area has a radius of curvature greater than the laminar flame thickness, most stretch occurs in more tightly curved flame elements.
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Keywords: Turbulent-combustion; Thin-reaction zones regime; Flame stretch; Direct numerical simulation

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1. Introduction

The so-called "thin reaction zones regime" of turbulent premixed combustion [1] delineates approximately a region of parameter space where disruption of the preheat zone by the penetration of small eddies occurs, but the thinner reaction zone is not significantly disturbed.

The length and time-scales of chemical and molecular transport processes in premixed flames are generally smaller than the length and time-scales on which affordable simulation of flames in practical geometries can be performed. Therefore, practical computational approaches rely on closure models for processes that cannot be explicitly represented in the simulation. For premixed combustion, several closure approaches exploit estimates of the total flame stretch to arrive at a final model. These include the G-equation approach for Reynolds averaged Navier–Stokes (RANS) simulation [1] or large eddy simulation

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(LES) [2], and the thickened flame approach [3] for LES. While the implementation of these approaches is substantially different, all can use an equilibrium assumption on the total flame stretch to arrive at a final expression for a "turbulent flame speed." The same approach can be used for an algebraic flame surface density model [4]. If the physics dictates that equilibrium is an inappropriate assumption, a balance equation for the flame surface density can be solved for RANS [5], or LES [6]. Alternatively, a balance equation can be solved for flame wrinkling [7]. In these approaches, the total flame stretch appears explicitly in the balance equation and requires closure.

In this work, data from direct numerical simulations (DNS) are used to evaluate current modelling concepts and assumptions for the propagation-curvature component of flame stretch. Particular attention is given to the modelling assumptions of Peters [1], which were explicitly derived for use in the thin reactions zone regime.

2. Models for flame stretch

Here, a flame is identified with a species mass fraction iso-surface. This approximation allows an unambiguous definition of the flame stretch and has served well in previous DNS studies.

The total stretch rate of a reactant species mass fraction iso-surface for the case of non-zero scalar gradient is given exactly by [8]

$$\dot{S} = a_t + s_d \nabla \cdot \mathbf{N}, \tag{1}$$

where a_t is the tangential strain rate, s_d is the displacement speed of the iso-surface relative to the flow (in the normal direction), $\mathbf{N}$ is the flame normal direction (pointing towards fresh gases), and so $\nabla \cdot \mathbf{N}$ is twice the mean curvature of the iso-surface. This work is focussed on the propagation-curvature component of stretch, $s_d \nabla \cdot \mathbf{N}$, which will be referred to henceforth simply as stretch. The term total stretch will be used to describe the sum of this term and tangential strain.

The iso-surface displacement speed is given by

$$s_d = -\frac{\mathrm{D}Y}{\mathrm{D}t} / |\nabla Y|, \tag{2}$$

where Y is the mass fraction of the species defining the surface. Assuming that the diffusive flux of ρY can be written as $\rho D \nabla Y$, where D is the species diffusivity, s_d can be decomposed in terms of three components [9]

$$s_d = s_{rr} + s_{ndf} + s_{tdf}. \tag{3}$$

These terms correspond to the effects of reaction s_{rr}, normal diffusion s_{ndf}, and tangential diffusion s_{tdf}, and are defined for a reactant species below:

$$\begin{aligned} s_{rr} &= -\frac{\omega}{\rho|\nabla Y|}, \\ s_{tdf} &= -D\nabla \cdot \mathbf{N}, \quad \text{and} \\ s_{ndf} &= -\frac{(\partial/\partial n)(\rho \mathrm{D}(\partial Y/\partial n))}{\rho|\nabla Y|}, \end{aligned} \tag{4}$$

where n is the distance in the normal direction and ω is the reaction rate.

Considering the propagation-curvature component of flame stretch, it is seen that Eqs. (3) and (4) result in

$$s_d \nabla \cdot \mathbf{N} = -D(\nabla \cdot \mathbf{N})^2 + (s_{rr} + s_{ndf})\nabla \cdot \mathbf{N}. \tag{5}$$

Tangential diffusion results in a term that is negative definite, always removing the flame area. As indicated by Peters [1], it is related to scalar dissipation. The other term can either be a production or destruction term depending on the local conditions.

The simplest model that can be assumed for the flame speed is that s_d is constant and equal to the value in a laminar flame, an assumption that has been traditionally made for flamelet approaches. In this case, the model for stretch is simply

$$s_d \nabla \cdot \mathbf{N} \approx s_{dL} \nabla \cdot \mathbf{N}, \tag{6}$$

where $s_{dL} = \rho_0 s_L / \rho$ is the value of s_d at the iso-surface in the unstrained laminar flame, ρ_0 is the density of the unburnt gas, and s_L is the unstrained laminar flame speed. This model will be referred to as the constant s_d model. Peters [1] refers to it as a kinematic restoration term.

For small and steady stretch, the flame speed is linearly dependent on the Markstein number Ma [10], and the stretch can be written as

$$s_d \nabla \cdot \mathbf{N} \approx s_{dL}(1 - Ma Ka) \nabla \cdot \mathbf{N}. \tag{7}$$

Here $Ka = \delta_L / s_L (a_t + s_L \nabla \cdot \mathbf{N})$, and δ_L is the unstrained laminar flame thickness. This model will be referred to as the small stretch model.

In the thin reaction zones regime, Peters [1] has argued that the tangential diffusion term is dominant due to large curvatures that are expected in this regime. Peters [1] also assumes that the components s_{rr} and s_{ndf} sum to a value of order of the laminar flame speed. For a quasi-steady curved flame, the flame speed is determined by diffusive-thermal effects influencing $s_{rr} + s_{ndf}$, and the stretch can be described by Eq. (7). However when the curvature is fluctuating, there is less time for diffusive-thermal effects to develop. Essentially, the argument made by Peters is that diffusive-thermal effects on these terms disappear in the limit of high frequency fluctuations, leaving a value that is close to the laminar flame speed. Asymptotic studies for small stretch [11] have provided some theoretical justification of this assumption. Computational studies of flames subjected to unsteady strain [12] and DNS computa-