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Consistent definitions of "Flame Displacement Speed" and "Markstein Length" for premixed flame propagation

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ABSTRACT

The definition of the flame displacement speed (FDS), often used to characterize the dynamical properties of premixed flames, is generally ambiguous because, except for a steadily propagating planar flame, the mass flow rate through the combustion region varies with distance through the flame and one is therefore faced with the difficulty of choosing a proper iso-surface to represent the flame surface. A directly related issue is the determination of the proportionality coefficient in the linear flame speed-flame stretch relation of weakly-stretched flames, known as the Markstein length, which depends strongly on the location inside the flame zone where it is measured or calculated. The objective of the present study is to identify an iso-surface and thereby a definition of the FDS that is well conditioned and less prone to uncertainties, and a consistent and unambiguous expression for the Markstein length. With a selected isotherm to represent the flame surface, the two most common definitions of the FDS are based either on the energy equation with the temperature as the progress variable, or on the kinematic characteristics of the surface (the propagation speed relative to the flow). In this study we examine the spherical flame geometry, a setup that provides an independent determination of the FDS that is not contingent upon an arbitrary selection of the flame surface and thus permits a proper evaluation of the two FDS definitions. A large number of simulations of premixed spherical propane/air flames with equivalence ratio ranging from 0.8 to 1.4 were carried out at various temperatures and pressures using both global single-step and detailed reaction schemes. Outwardly propagating spherical (or cylindrical) flames and inwardly propagating stationary spherical flames were examined. The dependence of the flame speed and flame temperature on stretch, and the corresponding Markstein length were identified for different isotherms selected to represent the flame surface, and the results were carefully compared to the asymptotic theory of weakly-stretched flames. The excellent agreement between theory and simulations provides a clear explanation and quantification of the differences found between the trends in the flame speed-flame stretch relation and the corresponding Markstein lengths, exhibited when the FDS was calculated based on an isotherm in the burned or unburned sides of the flame. We show that the proper isotherm for the evaluation of the FDS which is well-conditioned and properly accounts for the physics must be sufficiently close to the burned side of the flame. This choice is less prone to uncertainty, as the slope of the flame speed-flame stretch relation when reaching the burned side of the flame becomes less dependent on the selected iso-value. On the other hand, the choice of the fresh combustible mixture temperature as a reference location for the calculation of the FDS, and the corresponding unburned Markstein length, is ill conditioned and should be avoided.

1. Introduction

The *flame speed*, or *flame displacement speed*, defined as the propagation speed of a flame relative to the gas velocity is one of the most important characteristics of premixed combustion. It has a precise meaning when the flame is planar and propagates steadily because the mass flow rate through the flame is constant and the entire structure travels into the unburned mixture at a constant speed – the laminar flame speed S_L. For multi-dimensional and unsteady flows, the flame speed is a local property and its definition becomes ambiguous because the mass flow rate through the

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combustion region is not constant and varies with distance through the flame. Consequently, in order to investigate the flame dynamics, numerical simulations and experimental studies that resolve the finite thickness of the flame face the difficulty of choosing a proper iso-surface to represent the *flame surface*. An example, is the dependence of the flame speed on the stretch rate, which is a measure of the flame surface deformation resulting from its motion and from the underlying flow field. The relation between flame speed and flame stretch, which depends on the coupled flame-flow interactions is not generally known. For weakly-stretched flames, theoretical studies have shown that the flame speed-flame stretch relation is linear, and the proportionality coefficient is referred to as the Markstein length. Since the flame speed strongly depends on the iso-surface representing the flame surface, the concept of the Markstein length is equally ambiguous, which has resulted to confusion in the literature when applied to experimental and numerical data.

The notion of Markstein length originated from theoretical studies that treat the entire flame, consisting of the preheat and reaction zones, as a surface separating the hot combustion products from the fresh unburned mixture. This proposition dates back to the work of Darrieus [1] and Landau [2] on the stability of planar flames, where they assumed that the surface of the perturbed flame propagates relative to the unburned gas at a constant speed S_L. This assumption was later modified by Markstein [3] who introduced a dependence on the local curvature of the flame surface, through a phenomenological parameter that became known as the Markstein length. More recently, these ideas were solidified by rigorous asymptotic studies that exploited the disparity between the diffusion and hydrodynamic length scales associated with flame propagation, enabling the *derivation* of an expression for the flame speed by treating the flame as a thin, structured, internal layer [4–6]. Specifically, it is assumed that the flame thickness characterized by the diffusion length $l_f \equiv \mathcal{D}_{th}/S_L$, where $\mathcal{D}_{th}$ is the thermal diffusivity of the combustible mixture, is much smaller than the length scale L that characterizes the flow field. In the limit $l_f/L \to 0$, the entire flame shrinks to a surface – the flame front, which is uniquely determined, and an expression of the form

$$S_f = S_L - \mathcal{L}\mathbb{K} \tag{1}$$

was obtained for the (local) flame speed, namely, a linear dependence of the flame speed on the local stretch rate $\mathbb{K}$, which includes not only a curvature term as envisioned by Markstein, but also a dependence on the hydrodynamic strain experienced by the flame. The proportionality coefficient $\mathcal{L}$, which as noted earlier is known as the Markstein length, measures the sensitivity of the flame to the stretch rate, and depends on the fuel type and its reactivity, and on the mixture composition.

An important outcome of the asymptotic theory is the prediction that, when treated as a hydrodynamic discontinuity, the mass flux through the flame is not conserved with the difference accounting for accumulation within and transverse fluxes along the flame surface. As a result, the flame speed relative to the unburned and burned gases are not simply related by their density ratio. This was further exploited by Frankel and Sivashinsky [6] for spherically expanding flames, suggesting that the Markstein lengths calculated with respect to the unburned and burned gas are different. Distinct expressions for the burned and unburned Markstein lengths are also presented in [7] for constant properties, and generalized in [8,9] for temperature-dependent transport coefficients, arbitrary reaction orders, and stoichiometry.

The theoretical advances captivated the interest of experimentalists whose raw data from flame speed measurements of inwardly or outwardly spherically propagating flames and counterflow flames was found to correlate well with the linear relation (1). It has been consequently used to extract values of the laminar flame speed by extrapolating the data to zero stretch and/or to directly measure the Markstein length [10–20] in order to quantify stretch effects and incorporate them in studies of turbulent flames. However, the different experimental configurations and reference locations used to measure the flame speed by different groups led to differences on the trend followed by the variation of the flame speed with stretch that did not seem to fully agree with the theoretical predictions. In some cases an increasing/decreasing dependence of the flame speed on stretch was observed, depending on the mixture composition, while in other cases the same trend was observed for practically all mixtures. And, when the flame speed was extracted according to different definitions, both positive and negative dependence on stretch was observed for the same mixture. Moreover, extrapolating the data to zero stretch did not always converge to the laminar flame speed as expected. Indeed, it has been recognized by carefully examining the results of the asymptotic studies [21,22] that the reference location chosen for flame measurements is of major importance and could reconcile some of the observed differences.

As an alternative method to analyze the structure of stretched flames, an approximate integral approach was suggested in [23] with particular attention given to outwardly/inwardly propagating spherical flames, and modified in [24,25] in an attempt to extend the notion of flame stretch by accounting for the flame thickness. The integral approach requires estimating the fluxes into and out of a selected control volume, which in the aforementioned studies was based on physical arguments and previously derived elements of the asymptotic analysis, such as the existence of reaction-free convective–diffusive zone and a much thinner diffusive–reactive zone, and the exponential decay of the temperature and concentrations within the preheat zones. It is not surprising therefore that the expressions for the flame speed of stretched flames obtained using the integral approach have the same form as the asymptotic result (1), but the Markstein lengths, which depend on the adopted approximations, are quite different. For example, the expressions derived in [26] for the mass burning rate at various reference locations within the flame differ from those derived previously by asymptotic techniques [21,22], do not account for effects of stoichiometry and temperature-dependent transport and, as shown below, do not agree with results of direct numerical simulations.

Because of the ad hoc manner used to estimate the fluxes into and out of the flame, the integral analysis does not deal with the consistency requirements faced when carrying a rigorous asymptotic analysis, which led to erroneous claims about the validity of the integral analysis results; specifically that they are not necessarily limited to weak stretch and are valid for arbitrary Lewis numbers. It is evident, however, that neglecting transverse gradients and estimating the integrals involving the stretch-related terms using the unstretched flame solution [26], can be justified only for weak stretch. Moreover, the near-unity Lewis number distinguished limit, which is assumed in large activation energy asymptotic studies, is essential for the consistency of the analysis as clearly demonstrated in [27]; the resulting system obtained without invoking this assumption and known as "slowly-varying flames" has a pathological instability for all Lewis numbers. Indeed, the integral methodology lacks the rigor of the differential, asymptotic analysis, which as shown below, yields results that agree extremely well with numerical simulations. Nevertheless, it has some pedagogical merit and could be used in combination with numerical computations to incorporate effects due to complex reaction mechanisms and finite reaction layer thickness [25].

Numerical simulations, mostly concerned with spherically expanding/converging flames, have also shown that the flame displacement speed of weakly-stretched flames behaves generally as predicted by (1) but with slopes, or Markstein lengths, strongly dependent on the iso-surface selected to represent the flame. Some researchers [28,29] have used points close to the unburned end of