



# Determination of laminar flame speeds using stagnation and spherically expanding flames: Molecular transport and radiation effects



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## ABSTRACT

The uncertainties associated with the extraction of laminar flame speeds through extrapolations from directly measured experimental data were assessed using one-dimensional direct numerical simulations with focus on the effects of molecular transport and thermal radiation loss. The simulations were carried out for counterflow and spherically expanding flames given that both configurations are used extensively for the determination of laminar flame speeds. The spherically expanding flames were modeled by performing high fidelity time integration of the mass, species, and energy conservation equations. The simulation results were treated as “data” for stretch rate ranges that are encountered in experiments and were used to perform extrapolations using formulas that have been derived based on asymptotic analyses. The extrapolation results were compared then against the known answers of the direct numerical simulations. The fuel diffusivity was varied in order to evaluate the flame response to stretch and to address reactant differential diffusion effects that cannot be captured based on Lewis number considerations. It was found that for large molecular weight hydrocarbons at fuel-rich conditions, the flame behavior is controlled by differential diffusion and that the extrapolation formulas can result in notable errors. Analysis of the computed flame structures revealed that differential diffusion modifies the fluxes of fuel and oxygen inside the flame and thus affect the reactivity as stretch increases. Radiation loss was found to affect notably the extracted laminar flame speed from spherically expanding flame experiments especially for slower flames, in agreement with recent similar studies. The effect of radiation could be eliminated however, by determining the displacement speed relative to the unburned gas. This can be achieved in experiments using high-speed particle image velocimetry to determine the flow velocity field within the few milliseconds duration of the experiment. In general, extrapolations were found to be unreliable under certain conditions, and it is proposed that the raw experimental data in either flame configurations are compared against results of direct numerical simulations in order to avoid potential falsifications of rate constants upon validation.

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## 1. Introduction

The laminar flame speed,  $S_u^0$ , defined as the propagation speed of a steady, laminar, one-dimensional, planar, adiabatic flame is a fundamental property of any combustible mixture and it is a measure of the mixture's reactivity, diffusivity, and exothermicity. The accurate knowledge of  $S_u^0$  is essential towards validating kinetic models (e.g., [1]) and constraining uncertainties of rate constants [2]. Furthermore,  $S_u^0$  along with the Markstein length,  $L$ , which characterizes the response of laminar flame propagation to stretch, are inputs in turbulent flame models under conditions that the flamelet concept is applicable [3–5].

Measurement of  $S_u^0$  began as early as in the 1920s when Stevens [6,7] studied flame propagation at constant pressure by tracking spherically expanding flames, SEF, in a soap bubble filled with a flammable mixture. Since then, significant progress has been made both in the experimental and numerical determination of  $S_u^0$ . However, notable scatter by as much as 25 cm/s was persistent in published  $S_u^0$ 's of methane flames [8] until the 1980s when the effect of flame stretch [9] on flame propagation was accounted for and subtracted from the measurements reducing thus the experimental uncertainty notably [10–13]. Despite this progress, due to the relatively low sensitivity of  $S_u^0$  to chemical kinetics [14], there is need for experimental data with even lower uncertainty compared to what is reported currently so that they can be used for kinetic model validation.

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Among the various methods for measuring  $S_u^0$ , the counterflow flame, CFF, and the SEF configurations are well established and widely used, as they are considered to result in reliable data. Despite the fact that considerable effort has been devoted to understanding the intricacies and physics behind each approach, significant discrepancies persist in reported data, even when using the same method. Figure 1 depicts the relative deviation of experimental  $S_u^0$  with a normalized equivalence ratio  $\Phi \equiv \phi/(1 + \phi)$  [15], where  $\phi$  is the equivalence ratio, of *n*-heptane/air mixtures reported in different studies from the data of Ji et al. [16] that are used as the reference value. One can observe the increasing discrepancy between data obtained using the SEF [17] and CFF [18,19] configurations for off-stoichiometric  $\phi > 1$  mixtures; corrections of the data reported in Refs. [18,19] to account for the different unburned mixture temperatures,  $T_u$ , were made using the recommendation of Wu et al. [20]. It is evident that the disparity between the  $S_u^0$  data sets increases with  $\phi$  and this trend persists for flames of several high molecular weight, MW, fuels [16]. For  $\phi > 1$  hydrocarbon/air mixtures, air is abundant on both mass and molar basis compared to the fuel. Thus, the thermal diffusivity of the mixture is nearly that of nitrogen, and hence a Lewis number,  $Le$ , calculated based on oxygen, being the deficient reactant for  $\phi > 1$  mixtures, will be close to unity as shown in Fig. 2a regardless of the fuel MW. Yet, a high sensitivity of  $L$  to  $\phi$  has been reported, for example, for rich *n*-butane/air mixtures [21].

These inconsistencies point to possible uncertainties in the experimental determination of  $S_u^0$ , and could be associated with the reactant flow rates, i.e.  $\phi$ , diagnostic equipment, the flow velocity measuring approach, data analysis, and finally data interpretation. In order to tackle uncertainties associated with each experimental approach, detailed understanding of the physics controlling the flame behavior and response to fluid mechanics and loss mechanisms is required.

At pressures less than 10 atm,  $S_u^0$  can be measured using the CFF approach in which steady, laminar, and planar flames (e.g., [5,13]) are established. Under such conditions, the only parameter that can be varied for a given set of thermodynamic conditions is the flame stretch, and this effect can be characterized readily using available quasi-one dimensional codes (e.g., [22]).

Law and co-workers introduced the CFF approach to determine  $S_u^0$  [5,13,23]. The method involves the determination of the axial velocity profile along the system centerline and subsequently the identification of two distinct observables. A reference flame speed,  $S_{u,ref}$ , which is the minimum velocity just upstream of the flame, and a characteristic stretch,  $K$ , which is the maximum absolute

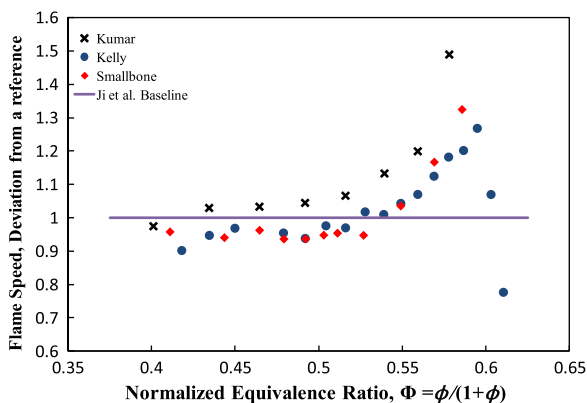


Fig. 1. Deviation of experimental  $S_u^0$ 's of *n*-heptane/air mixtures at  $p = 1$  atm from that of Ji et al. [16] ( $T_u = 353$  K) represented by the solid line. Data represented by symbols include: (•) Kelley et al. [17] ( $T_u = 353$  K), (•) Smallbone et al. [18] ( $T_u = 350$  K) and (X) Kumar et al. [19] ( $T_u = 360$  K).

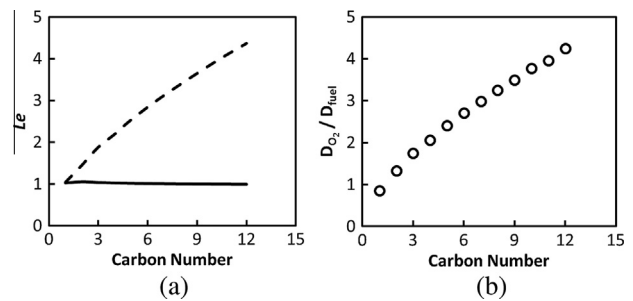


Fig. 2. (a) Variation of  $Le$  with carbon number for *n*-alkane/air mixtures at  $p = 1$  atm and  $T_u = 298$  K, for  $\phi = 0.7$  (dashed line) and  $\phi = 1.4$  (solid line). (b) Variation of the ratio of oxygen diffusivity to fuel diffusivity with carbon number for  $\phi = 1.4$  *n*-alkane/air mixtures at  $p = 1$  atm and  $T_u = 298$  K.

value of the axial velocity gradient in the hydrodynamic zone. Thus, by varying  $S_{u,ref}$  with  $K$  in the experiments, it was proposed [5,13,23] that  $S_u^0$  can be determined by performing a linear extrapolation of the experimental data to zero stretch given that as  $K \rightarrow 0$ ,  $S_{u,ref}$  should degenerate to  $S_u^0$ . This approach was used in several studies (e.g., [24–26]) for  $H_2$  and  $C_1$ – $C_2$  hydrocarbon flames.

Subsequently, Tien and Matalon [27] demonstrated through asymptotic analysis that the  $S_{u,ref}$  vs.  $K$  response is non-linear as  $K \rightarrow 0$ , and that linear extrapolation of  $S_{u,ref}$  to  $K = 0$  results in the over-estimation of  $S_u^0$ ; it should be noted that  $S_{u,ref}$  is not the stretched flame speed,  $S_u$ , as it is affected by thermal dilatation and flow divergence effect [13,27,28]. Tien and Matalon [27] produced also a non-linear expression describing the variation  $S_{u,ref}$  with  $K$ , which subsequently was expressed by Davis and Law [29] in a more compact way as:

$$S_{u,ref} = S_u^0 \{1 - (\mu - 1)Ka + Ka \ln[(\sigma - 1)/Ka]\}. \quad (1)$$

In Eq. (1),  $\mu$  is the Markstein number,  $Ka \equiv \alpha K / (S_u^0)^2$  the Karlovitz number,  $\alpha$  the thermal diffusivity of the mixture, and  $\sigma \equiv (\rho_u / \rho_b)$  with  $\rho_u$  and  $\rho_b$  being the densities of the unburned and burned states at equilibrium respectively.

Chao et al. [30] used asymptotic analysis to show that the error introduced by linear extrapolations can be reduced for small  $Ka$  and large burner separation distance relative to the flame thickness. Vagelopoulos et al. [31] further showed computationally and experimentally that in order for the linear extrapolation to be accurate,  $Ka$  must be of the order of 0.1 for  $CH_4$ /air,  $C_3H_8$ /air, and lean  $H_2$ /air flames.

Recently, Egolfopoulos and co-workers [16,32,33] introduced a computationally assisted approach in quantifying the non-linear variation of  $S_{u,ref}$  with  $K$ . Specifically, direct numerical simulations (DNS) of the experiments are carried out with detailed description of molecular transport and chemical kinetics to avoid simplifying assumptions used in asymptotic analysis. Thus, the variation of  $S_{u,ref}$  with  $K$  is computed and can be used to perform the non-linear extrapolations of the experimental data; indeed the DNS approach reproduces the non-linear behavior of  $S_{u,ref}$  with  $K$  as predicted by Tien and Matalon [27]. Given that the computed  $S_{u,ref}$  vs.  $K$  curve may lie over or below the data due to transport and kinetic model uncertainties, it was shown that as long as the discrepancies between data and predictions are not large, say within 30–40%, the shape of the  $S_{u,ref}$  vs.  $K$  curve is minimally affected and could be translated to best fit the data and derive  $S_u^0$  at  $K = 0$ . This was confirmed through DNS in which the rates of main  $H + O_2 \rightarrow OH + O$  branching or  $CO + OH \rightarrow CO_2 + H$  oxidation reactions as well as the diffusion coefficients of the reactants were modified intentionally by as much as 30–40%. It was shown that even under such notable but not excessive modifications of the overall reaction

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