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Uncertainty reduction in laminar flame speed extrapolation for expanding spherical flames

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ABSTRACT

The quantification and reduction of the uncertainties in the extrapolation process in laminar flame speed measurements were studied using expanding spherical flames under positive Markstein length ($L_b > 0$) conditions. The experimental and computational results were first compared showing their differences. The performance of three extrapolation formulas was then examined under a wide range of experimental conditions using various extrapolation ranges and pressures. It is found that the extrapolation uncertainty contains two sources of error, namely model error and random error. The individual effects of the upper and lower bounds of the extrapolation range under various L_b conditions were studied and the ratio of L_b and the flame radius range is found to be the controlling parameter of the model error. Small value of $|L_b/R_f|$ allows the neglect of the model error by increasing the upper or the lower bound of the flame radius range. A new empirical parameter, $L_b/R_{f,new}$, was defined according to the experimental results, while it is recognized that the random error is mainly affected by the number of points for extrapolation and that at least 30 points should be used to remove the random error.

1. Introduction

The laminar flame speed, $S_u{}^0$, being one of the most important global properties of a combustible mixture, is defined as the speed relative to the unburned gas, with which a planar, one-dimensional flame front adiabatically propagates normal of its surface in the doubly infinite domain [1]. An accurate knowledge of its value not only is of practical utility in the assessment of the mixture's burning rate and flammability, it can also be used to develop and validate combustion chemistry as well as to advance our understanding of flame dynamics. Several flame configurations have been used to measure $S_u{}^0$, such as the Bunsen flame, the flat-burner flame, the counter-flow flame and the expanding spherical flame [2]. Since none of these flames conforms to the idealized situation of laminar flame propagation, based on which $S_u{}^0$ is defined, with the measured flame speeds being affected by system effects such as aerodynamic stretch and heat loss, it is essential that these measured flame speeds be extrapolated to that corresponding to vanishing values of the system effects to yield the "true" laminar flame speed. Consequently, the accuracy of the extrapolation procedure directly affects the fidelity of the laminar flame speed eventually determined.

Among the various techniques mentioned above for the determination of laminar flame speeds, the expanding spherical flame has been demonstrated to be highly versatile, having the potential to offer data of good accuracy, especially at elevated pressures, which are typically not accessible using other configurations. Consequently, recently there has been substantial interest towards reducing the uncertainty in the extrapolation involving expanding spherical flames so as to further enhance the fidelity of the procedure [3,4]. To this end we note that among the various theoretically derived linear and nonlinear stretch extrapolation formulas [3,5–7], three have been extensively employed,

$$\text{Linear Stretch (LS)}: S_b = S_b^0 - L_b k \tag{1}$$

$$\text{Linear Curvature (LC)}: S_b = S_b^0 - 2S_b^0 L_b / R_f \tag{2}$$

$$\text{Nonlinear Quasi-steady (NQ)}: \ln(S_b) = \ln\left(S_b^0\right) - 2S_b^0 L_b / (R_f S_b) \tag{3}$$

where R_f is the flame radius, $S_b = dR_f/dt$ is the stretched flame speed, $k = 2S_b/R_f$ the stretch rate and L_b the Markstein length that characterizes the variation in the local flame speed due to the influence of stretch. The first relation, denoted as LS, indicates that the stretched flame speed S_b varies linearly with the local stretch

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rate [8]. The second relation, denoted as LC, states that S_b varies linearly with the flame curvature $1/R_f$. It was first proposed by Markstein [9] and rigorously derived by Frankel and Sivashinsky [10]. The third, non-linear, relation, denoted as NQ, is based on the assumption that the flame is weakly stretched, and propagates in a quasi-steady manner. NQ was first derived by Ronney and Sivashinshy [11] and then used and explored by Kelley and Law [6], Halter et al. [12] and Chen [5].

To compare the degree of accuracy of these expressions, the extrapolation formulas of LS, LC and NQ are expanded using the Taylor expansion to the third term in terms of the perturbation L_b/R_f, which is a smaller number since L_b is of the same order with flame thickness and the flame size is much larger than the flame thickness during extrapolation [7]

$$\mathrm{LS}: S_b/S_b^0 = 1 - 2L_b/R_f + 4\left(L_b/R_f\right)^2 + O\left(L_b/R_f\right)^3 \tag{4}$$

$$\mathrm{LC}: S_b/S_b^0 = 1 - 2L_b/R_f \tag{5}$$

$$\mathrm{NQ}: S_b/S_b^0 = 1 - 2L_b/R_f - 2\left(L_b/R_f\right)^2 + O\left(L_b/R_f\right)^3 \tag{6}$$

It is then seen that the three expressions have the same first-order expansion, while start to show differences in the second-order term, $(L_b/R_f)^2$. Consequently the relevant nondimensional parameter controlling the accuracy of the extrapolation procedures is the ratio of the Markstein length and the flame radius used for extrapolation, i.e. L_b/R_f, and the model differences can be ignored when the value of $|L_b/R_f|$ is small. The Markstein length L_b is an intrinsic parameter of a mixture and is of the order of flame thickness, being fundamentally affected by the fuel type, the equivalence ratio, and the system pressure.

In addition to the degree of expansion, it is also desirable to expand the range of the flame radius as much as possible so as to include as many data points as possible in order to reduce the random error. Consequently, the upper bound of the flame radius range, $R_{f,U}$, should be made as large as possible, but without triggering flame front instability as well as confinement effects from the chamber walls; while the lower bound, $R_{f,L}$, should be as small as possible but without incurring ignition effects including those of the electrodes. Furthermore, in studying the $R_{f,U}$ effect on extrapolation, Chen [5] theoretically found that while the extrapolation formulas differ substantially at small flame radii, they all converge at larger $R_{f,U}$. In the numerical study of Jayachandran et al. [13], increasing $R_{f,U}$ by a factor of five was found to result in considerably improved prediction of the laminar flame speeds for rich C_2H_4/air and n-C_7H_{16}/air flames. The $R_{f,L}$ effect on the extrapolation has not been studied as much as that for the $R_{f,U}$ effect. Halter et al. [12] experimentally found that for the CH_4/air flame at $\phi = 1.3$, the relative difference of $S_u{}^\circ$ extracted from linear and nonlinear formulas can be reduced from 21% to 0.6% if $R_{f,L}$ is increased from 0.8 cm to 2.0 cm. To investigate the coupling effect of L_b and R_f on extrapolation, Wu et al. [3] took the mid-point of the flame radius range $R_{f,mid}$ to represent the entire flame radius range, with $R_{f,L}$ fixed at 1 cm. The extrapolation uncertainty shows scattering based on $L_b/R_{f,mid}$ in their computational results, indicating that $L_b/R_{f,mid}$ may not be suitable to represent L_b/R_f. In summary, since the previous studies have mainly focused on simulations, experimental validation is needed. Furthermore, the use of L_b/R_f as the controlling parameter of extrapolation uncertainty also needs to be systematically investigated by experiments, especially at various pressures and under Lewis number, $Le > 1$, conditions.

In light of the above considerations, the present work aims to: (1) validate the importance of L_b/R_f on extrapolation under various experimental conditions; (2) complement the previous results by investigating the individual effects of L_b and R_f on extrapolation; (3) identify an alternate characteristic flame radius to replace $R_{f,mid}$ in L_b/R_f. In the following, we shall briefly describe our experimental setup, in Section 2. Experimental and numerical results are then compared in Section 3, followed by the effects of L_b and R_f on extrapolation, in Sections 4 and 5, respectively. A new empirical parameter $L_b/R_{f,new}$ is proposed in Section 6. Conclusions are given in Section 7.

2. Experimental methodology

Since the uncertainty in the extrapolation process is mainly controlled by L_b/R_f, it is important to overcome the limitation of R_f in experiments and to achieve a wide range of L_b/R_f for investigation. In this work, both the ranges of R_f and L_b have been substantially extended with a new and larger experimental design for the study of spherically expanding flames.

2.1. Experimental setup

To extend the range of R_f, a Generation-3 constant-pressure dual-chamber spherical flame apparatus, with a larger chamber size and therefore larger useful extrapolation ranges, is used. Since this is the first report using this new facility, we discuss in moderate detail its specifications. The schematics are shown in Fig. 1. The system consists of two concentric chambers. The outer chamber is cylindrical while the inner chamber has a spherical internal surface allowing for tighter isotropy than the cylindrical chambers. The inner diameter of the inner chamber is 250 mm. In the experiments, the two chambers are initially partitioned from one another by four groups of switch valves with holes that are off-set from each other. The inner chamber is filled with a mixture of fuel and oxidizer based on partial pressures, while the outer chamber is filled with an inert. During the filling process, the pressure difference between the inner and outer chambers is measured with differential pressure transducer so as to ensure that the pressure difference stays small. After finishing the filling process, a mixing pump is used to mix the fuel and air in the inner chamber by taking the combustible mixture out of the inner chamber from one end and then sending it back through the other end. The ignition starts after several minutes of waiting time to ensure homogeneity and quiescence of the mixture in the inner chamber. Centrally located electrodes are used to ignite the mixture in the inner chamber as soon as the switch valves open and the inner and outer chambers are connected.

Two quartz windows with 160 mm in diameter are located at two sides of the vessel for optical access. The history of the flame radius, $R_f(t)$, is imaged using Schlieren photography and recorded with a high-speed digital motion camera (Photron Fastcam SA-Z) at 8000–20,000 frames per second, depending on the flame speed of the mixture. Schlieren images from a typical experiment are shown in Fig. 2. The spatial resolution of the camera is roughly 0.2 mm/pixel. The purities of the fuels in the present experiments (H_2 and C_3H_8) exceed 99.9%, specifically 99.995% and 99.95%, respectively. All experiments are repeated and the repeatability error is less than 3% considering the relative difference in the extracted laminar flame speeds from different runs using the same extrapolation model and flame radius range. It should be noted that one does not need to consider the repeatability error when assessing the extrapolation uncertainty since the experimental data from the same runs are used for different extrapolation procedures. The overall experimental uncertainty in the extrapolated laminar flame speeds contains both the repeatability error and the extrapolation uncertainty. Furthermore, it is found in this work, shown in the Supplementary material, that the ignition effect is negligible beyond $R_f = 0.7$ cm, which is quite similar to those in previous studies [14, 15]. So the minimum $R_{f,L}$ is conservatively selected at 1 cm. The maximum $R_{f,U}$ is selected at 4 cm, which is smaller than 40%