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On the accuracy of laminar flame speeds measured from outwardly propagating spherical flames: Methane/air at normal temperature and pressure

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ABSTRACT

The present work investigates the accuracy of laminar flame speeds measured from outwardly propagating spherical flames. We focus on methane/air mixtures at normal temperature and pressure, for which there is a variety of data sets reported in the literature. It is observed that there are large discrepancies in laminar flame speed measurement, which makes these experimental data unhelpful for restraining the uncertainty of chemical models. Different sources of uncertainty/inaccuracy (including mixture preparation, ignition, buoyancy, instability, confinement, radiation, nonlinear stretch behavior, and extrapolation) are discussed and their contributions to large discrepancies in laminar flame speed measurement are assessed with the help of 1-D simulation. It is found that the uncertainty in equivalence ratio can bring large inconsistency in laminar flame speed measurement, especially for off-stoichiometric mixtures and experiments using pressure gauge with normal or low accuracy. For fuel-rich methane/air mixtures, the large deviations in laminar flame speed measurement could be partly caused by nonlinear stretch behavior and extrapolation. The change of the influence of different sources of uncertainty with initial pressure, initial temperature, and fuel carbon number is also discussed. Furthermore, it is shown that the discrepancy in raw experimental data can be possibly hidden after extrapolation is conducted. Therefore, the data used for extrapolation as well as extracted results should be reported and compared with simulation or other experiments. The recommendations on the laminar flame speeds measurement using the propagating spherical flames are also provided.

1. Introduction

The laminar flame speed, S_u^0, is defined as the speed at which a planar, unstretched, adiabatic, premixed flame propagates relative to the unburned gas [1]. It is an important parameter of a combustible mixture since it determines the fuel burning rate and flame stabilization in practical combustors. On a more fundamental level, S_u^0 is an important target for validating chemical mechanisms and for developing surrogate fuel models (e.g., [2–7]). Various experimental approaches have been developed to measure S_u^0 using different flame configurations such as Bunsen flame, flat-burner flame, counterflow/stagnation flame, and outwardly propagating spherical flame (OPF) [1,5]. The advantages and limitations of these approaches have been recently reviewed by Egolfopoulos et al. [5]. Currently, due to the simple flame configuration and well-defined stretch rate, the OPF method is popularly used to measure S_u^0, especially at high pressures.

Accurate measurement of laminar flame speed is extremely important since the sensitivity of S_u^0 to chemical kinetics is relatively low [5]. It is very difficult to constrain the uncertainty of chemical models using low-quality (with large-uncertainty) experimental data of S_u^0 [5,8]. Recently, substantial attention has been devoted to improving the accuracy of laminar flame speed measurement using the OPF method ([5] and references therein). For example, a collaborative study has been initiated to investigate the potential error sources and to reduce the uncertainty associated with S_u^0 measurement [9]. For large molecular weight fuels or liquid fuels, the uncertainty associated with S_u^0 measurement using the OPF method can be large due to the effects of molecular transport (differential diffusion of reactants) [10] and/or fuel heating and vaporization [5,9]. For small molecular weight gaseous fuels (such as methane and propane, not including hydrogen), the uncertainty in S_u^0 measurements is usually considered to be small, at least for conditions at normal temperature and pressure (NTP, $T_u = 298$ K, $P = 1$ atm). A new experimental setup for S_u^0 measurement is usually

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validated against experimental data for CH_4/air at NTP reported in the literature.

However, as will be shown in this study (see Figs. 1 and 3), the discrepancies in S_u^0 measured for CH_4/air at NTP using the OPF method still remain substantial – often exceeding typical quoted uncertainties in the measurements. These persistent discrepancies among experimental data themselves make it difficult to interpret comparisons between experimental data and model predictions in kinetic mechanism validation [8]. In order to reduce the discrepancies in S_u^0 measurements, the possible sources of uncertainty should be investigated. Besides, information on the uncertainty in S_u^0 measured in experiments is also important for kinetic model validation and optimization [11,12].

The objectives of the present work are (1) to identify the discrepancies in S_u^0 measured for CH_4/air at NTP using the same OPF method by different groups; and (2) to investigate possible sources of uncertainty/inaccuracy in S_u^0 measurements. Specifically, a variety of experimental data sets for CH_4/air reported in the literature [13–26] is collected to show the differences in S_u^0 measurement using the OPF method. Moreover, effects of mixture preparation [5,9,27,28], ignition [29–32], buoyancy [33,34], instability [35–37], confinement [38–41], radiation [9,10,41–44], nonlinear stretch behavior [22,45–49], and extrapolation [50,51] on the discrepancies in S_u^0 measurement are examined based on 1-D simulation of propagating planar and spherical flames. It should be noted that Egolfopoulos et al. [5] have recently reviewed possible sources of uncertainty in S_u^0 measurement using the OPF method. However, in that study the contributions of individual source of uncertainty have not been assessed/quantified specifically for CH_4/air.

The paper is organized as follows: in Section 2, the OPF method and numerical method are briefly described; then, in Section 3, discrepancies in S_u^0 measured by different groups for CH_4/air at NTP are presented; possible sources of uncertainty in S_u^0 measurement using the OPF method are discussed in Section 4, after which additional notes and recommendations are respectively presented in Sections 5 and 6; and finally, the conclusions are summarized in Section 7.

2. Methodologies

Depending on the combustion chamber design and pressure rise, there are two different methods for S_u^0 measurement using OPF: the constant-pressure method (e.g., [13–26]) and the constant-volume method (e.g., [52–54]). Only the constant-pressure OPF method is considered here and hereafter it is simply called OPF method. In this method, a confined chamber or a pressure-release dual-chamber is used in experiments. The flame front history of OPF, $R_f = R_f(t)$, is recorded by high-speed schlieren or shadowgraphy. Usually, the burned gas inside the spherical flame is assumed to be static and thus the stretched flame speed relative to burned gas is $S_b = dR_f/dt$. The unstretched laminar flame speed, S_b^0, together with the Markstein length, L_b, both relative to burned gas, can be obtained from extrapolation based on the following linear model:

$$S_b = S_b^0 - L_b K \tag{1}$$

where $K = (2/R_f)(dR_f/dt)$ is the stretch rate for OPF. Knowing S_b^0, S_u^0 can be determined through $S_u^0 = \sigma S_b^0$, where $\sigma = \rho_b/\rho_u$ is the density ratio between burned gas (at equilibrium condition) and unburned gas.

When Eq. (1) is used, numerical differentiation needs to be conducted to get S_b and K. This can be avoided by integrating Eq. (1) which yields the following expression:

$$S_b t = S_b^0 t - 2L_b \ln(R_f) + \text{const} \tag{2}$$

Besides the linear model, the following nonlinear model was proposed by Kelley and Law [45] in the extraction of S_b^0 and L_b:

$$\left(\frac{S_b}{S_b^0}\right) \ln\left(\frac{S_b}{S_b^0}\right) = -\frac{2L_b}{R_f} \tag{3}$$

This model is based on the quasi-steady, adiabatic form of the relation first derived by Ronney and Sivashinsky [55]. The accuracy and performance of the nonlinear model were discussed in [22,45–47].

This paper summarizes the experimental data for CH_4/air at NTP from previous studies [13–26] which measured S_u^0 using the OPF method. The details on initial temperature and pressure, equivalence ratio range, extrapolation model, and chamber geometry are summarized in Table 1 (Most of data sets in the table were reported in the last ten years).

In order to isolate and assess the contribution of individual source of uncertainty, 1-D simulation of propagating planar and spherical flames is conducted. Detailed chemistry for methane oxidation, GRI-Mech. 3.0 [56], is used in simulation. The unstretched, adiabatic, freely-propagating planar flame is simulated using CHEMKIN-PREMIX code [57] to get S_u^0 and σ. The number of grid points is kept to be above 700 so that the calculated laminar flame speed and density ratio is grid-independent. OPF is simulated using A-SURF [31,41], which solves the conservation equations of one-dimensional, multi-component, reactive flow in a spherical coordinate using the finite volume method. The CHEMKIN packages [58] are incorporated into A-SURF to calculate the temperature- and component-dependent thermodynamic and transport properties. Detailed chemistry is efficiently handled in A-SURF with the help of algorithms introduced in [59,60]. A-SURF has been successfully used in previous studies on ignition and flame propagation (e.g., [61–64]). The details on governing equations, numerical schemes, and code validation can be found in [31,41]. To adequately resolve the moving flame front, a multi-level, dynamically adaptive mesh with finest mesh size of 8 μm is used. Unless otherwise stated, a large chamber radius of $R_W = 100$ cm is used (to ensure the confinement effect is negligible) and adiabatic condition is considered (to eliminate the radiation effect).

3. Discrepancies in S_u^0 measured for CH_4/air at NTP

The laminar flame speeds of CH_4/air at NTP measured by different groups [13–26] (see Table 1) are plotted in Fig. 1. The prediction from GRI-Mech. 3.0 [56] is also shown for comparison. All the experimental results (symbols in Fig. 1) were measured using the OPF method. Lower scatter is observed for stoichiometric mixture, and higher scatter is observed for off-stoichiometric mixtures. Even for near-stoichiometric mixture of $\phi = 0.9$, high scatter is observed. It is noticed that S_u^0 measured near the lean flammability limit by Wang et al. [23] is much lower than prediction from GRI-Mech. 3.0. This is not caused by buoyancy effect since Wang et al. [23] conducted experiments at 10^{-3}–10^{-2} g reduced gravity. It is the radiation and compression effects that make reported S_u^0 much lower than its correct value [41].

The Markstein lengths of CH_4/air at NTP measured using the OPF method are shown in Fig. 2. Compared to S_u^0, the discrepancies in L_b are shown to be much larger. The relative difference can even be above 300% under fuel-rich conditions. This is due to the facts that L_b measurement is very sensitive to extrapolation and that the uncertainty in L_b is about one-order larger than that in S_u^0 [46]. Significant effort needs to be devoted to improving the