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Radiation-induced uncertainty in laminar flame speed measured from propagating spherical flames

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ABSTRACT

Laminar flame speeds measured using the propagating spherical flame method are inherently affected by radiation. Under certain conditions, a substantial uncertainty in laminar flame speed measurement is caused by radiation, which results in a great concern for kinetic mechanism validation and development. In this study, numerical simulations with detailed chemistry and different radiation models are conducted to examine the effects of radiation on spherical flame propagation. The emphasis is placed on quantifying the uncertainty and corrections associated with radiation in laminar flame speed measurements using propagating spherical flames. The radiation effects on flame speeds at normal and elevated temperatures and pressures are examined for different fuel/air mixtures including methane, propane, iso-octane, syngas, hydrogen, dimethyl ether, and n-heptane. The radiative effects are conservatively evaluated without considering radiation reflection on the wall. It is found that radiation-induced uncertainty in laminar flame speeds is affected in the opposite ways by the initial temperature and pressure. An empirical correlation quantifying the uncertainty associated with radiation is obtained. This correlation is shown to work for different fuels at normal and elevated temperatures and pressures. Therefore, it can be directly used in spherical flame experiments measuring the laminar flame speed. Furthermore, a method to obtain the radiation-corrected flame speed (RCFS) is presented and it can be used for laminar flame speed measurement using the propagating spherical flame method.

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. It is one of the most important parameters of a combustible mixture. Accurate determination of S_u^0 is important for developing and validating chemical mechanisms and surrogate fuel models [1–4], especially at high pressure [5]. Predictions of S_u^0 can be easily obtained through simulating one-dimensional, planar, adiabatic, premixed flames (e.g. using PREMIX code) with chemical models. However, in experiments it is very difficult to establish a planar, unstretched, adiabatic flame and different flame configurations (such as outwardly propagating spherical flame, counterflow or stagnation flame, and Bunsen flame) have been used to measure S_u^0. Different effects such as stretch, flow compression, and heat loss must be subtracted from the experimental data in order to unambiguously determine S_u^0. Several experimental approaches have been developed to measure S_u^0. Currently, due to the simple flame configuration and well-defined stretch rate, the propagating spherical flame method is popularly used to measure S_u^0 (e.g., [6–15]). In this method, a quiescent homogeneous premixture in a closed chamber is ignited at the center and the ignition kernel evolves into an outwardly propagating spherical flame. The flame front history, $R_f = R_f(t)$, is recorded by using high-speed schlieren or shadowgraphy. Usually the stretched flame speed relative to burned gas, S_b, is first obtained from flame front history and extrapolated to zero stretch rate to get the unstretched laminar flame speed, S_b^0, relative to burned gas. Then 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 the burned gas (at adiabatic equilibrium condition) and unburned gas [6–15].

However, there still exist considerable discrepancies in the laminar flame speeds measured by different researchers using propagating spherical flames at the same conditions – sometimes

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exceeding typical quoted uncertainties in the measurements [4,16,17]. Therefore, substantial attention has been devoted to obtaining accurate S_u^0 from propagating spherical flames. For examples, the effects of ignition and unsteady transition [18–20], buoyancy [21], flow compression and finite chamber confinement [22,23], flame instability [24], and nonlinear extrapolation [25–28] have been examined recently.

Radiation is another process which can significantly modify the flame propagation speed and limits via radiation heat loss and radiation absorption [29–31]. In spherical flame experiment, radiation of H_2O and CO_2 in the burned gas region cannot be avoided and affects the speed of flame propagation. Therefore, all laminar flame speed data measured using the propagating spherical flame method are inherently affected by radiation. However, radiation effects are usually neglected in experiments [6–15]. In fact, it is difficult to quantify the correction in S_u^0 associated with radiation due to its nonlinear character, though in the literature there are many theoretical studies (e.g., [32–35]) investigating radiation effects on spherical flame propagation. Recently, radiation effects on laminar flame speed measurement using the propagating spherical flame method have drawn attention from researchers. Taylor and coworkers [6,36] first analyzed the flame speed measurement error in spherical flames due to thermal radiation and found that the radiation-induced reduction in S_u^0 is less than 5% under worst-case conditions. Chen et al. [37] and Qiao et al. [38] assessed radiation (re)absorption effects on spherical flame propagation and concluded that quantitative prediction of flame speed of CO_2 diluted mixtures requires an accurate spectral dependent radiation model. Chen [39] studied radiation effects on methane/air flames near the lean flammability limit. It was found that radiation reduces the flame temperature and induces inward flow of burned gas, both of which slow down the flame propagation. Radiation was shown to cause up to 25% under-prediction of S_u^0. Beeckmann et al. [40] and Jayachandran et al. [41] found that radiation cannot be neglected even for mixtures not close to the flammability limits. Santner et al. [42] conducted a semi-analytical investigation of radiation heat loss on the uncertainty of S_u^0 measured at high pressure. They demonstrated that the high pressure flame speeds of H_2/He/O_2 are only slightly affected by radiation.

Since uncertainty quantification for laminar flame speed measured in experiments is crucial to kinetic model development and optimization [44,45], accurate determination of uncertainty in S_u^0 associated with radiation is very important [42]. However, in studies [36–42] mentioned above, radiation-induced uncertainty in S_u^0 was not quantitatively assessed or was assessed only for certain types of fuel/air mixtures. There is no general correlation for radiation-induced uncertainty in S_u^0 which can be directly used in laminar flame speed measurements by the propagating spherical flame method. Therefore, the first objective of this study is to provide a general quantification of the uncertainty in S_u^0 associated with radiation for different fuel/air mixtures.

Except the work of Ju and coworkers [37,42] and Jayachandran et al. [41] which considered radiation effects at elevated pressures, the previous studies were all focused on spherical flames at normal temperature and pressure (NTP). It is not clear how the initial temperature and pressure affect radiation-induced uncertainty in S_u^0 measured from propagating spherical flames. Therefore, the second objective is to evaluate the radiation effects at elevated temperature and pressure and to find the change of radiation-induced uncertainty in S_u^0 with the initial temperature and pressure.

In kinetic model validation and optimization, usually the predicted adiabatic laminar flame speeds are used. To compare results predicted by kinetic models with those from measurements using propagating spherical flames, radiation-correction must be conducted to account for a decrease in laminar flame speed due to radiative loss. The third objective of this study is therefore to get the radiation-corrected flame speed (RCFS).

Based on the objectives discussed above, direct numerical simulations are conducted to examine the effects of radiation on spherical flame propagation and to quantify uncertainty and corrections associated with radiation in laminar flame speed measurement for different fuels in air at a variety of temperatures, pressures, and equivalence ratios. An empirical correlation for uncertainty in S_u^0 associated with radiation is obtained. It works for different fuels at normal and elevated temperatures and pressures and can be directly used in laminar flame speed measurements using the propagating spherical flame method.

The paper is organized as follows: in Section 2, numerical methods and specifications are presented; then, in Section 3, radiation effects on spherical flame propagation are briefly described; radiation-induced uncertainty/reduction in laminar flame speed measurement are quantified in Section 4, based on which the method to get RCFS is proposed in Section 5; and finally, the conclusions are summarized in Section 6.

2. Numerical methods and specifications

One-dimensional outwardly propagating spherical flames are simulated using the in-house code for Adaptive Simulation of Unsteady Reacting Flows (A-SURF) [19,39]. The conservation equations for a multi-species reactive flow are solved by using the finite volume method [19,39]. The CHEMKIN packages [46] are incorporated into A-SURF to calculate the temperature- and component-dependent thermodynamic and transport properties. A-SURF has been successfully used in previous studies on ignition and spherical flame propagation (e.g., [47–51]). The details on governing equations, numerical schemes, and code validation can be found in [19,39].

Three radiation models are employed so that the radiation effects can be quantified through comparison between results predicted by different models. These models are summarized in Table 1: the first one is the adiabatic model (denoted by 'ADI') in which radiation is neglected; the second one is the optically thin model (denoted by 'OTM') in which only radiation emission from CO_2, H_2O, CO, and CH_4 is considered [29]; and the third one is the statistical narrow band model (denoted by 'SNB') in which a fitted statistical narrow-band correlated-*k* (FSNB-CK) method [37] is employed to calculate radiative transport including both emission and re-absorption. The Planck mean coefficients in the OTM model were derived from the SNB model in the optically thin limit [29]. Detailed validation of the SNB model for H_2O and CO_2 radiation can be found in [43]. It was shown in Ref. [37] that the SNB model reproduces the theoretical radiation flux at hollow sphere boundaries and the measured flame speed. However, the OTM under-predicts the flame speed since radiation loss is over-predicted. The drawback of the OTM is that it over-predicts the radiative loss and is less accurate than the SNB model. The disadvantage of the SNB model is that it takes much more computational time than the OTM.

We consider several types of fuel: methane, propane, iso-octane, syngas (with five different H_2/CO ratios: 5/95, 10/90, 25/75, 50/50, and 100/0), dimethyl ether (DME), and n-heptane.

Table 1
Three models for radiation.

Abbreviation	Model description
ADI	Adiabatic model without radiative loss
OTM	Optically thin model; only radiative emission is considered
SNB	Statistical narrow band model; radiative emission and absorption are considered

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