Combustion and Flame 000 (2015) 1–14

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Laminar flame speeds under engine-relevant conditions: Uncertainty quantification and minimization in spherically expanding flame experiments

Christodoulos Xiouris, Tailai Ye, Jagannath Jayachandran, Fokion N. Egolfopoulos*

Department of Aerospace and Mechanical Engineering University of Southern California, Los Angeles, CA 90089-1453, USA

ARTICLE INFO

Article history:
Received 8 July 2015
Revised 1 October 2015
Accepted 2 October 2015
Available online xxx

Keywords:
Flame propagation
Laminar flame speed
Uncertainty quantification
Flame kinetics
Engine conditions

ABSTRACT

The spherically expanding flame method is the only approach for measuring laminar flame speeds at thermodynamic states that are relevant to engines. In the present study, a comprehensive evaluation of data obtained under constant pressure and constant volume conditions was carried out through experiments, development of a mathematically rigorous method for uncertainty quantification and propagation, and advancement of numerical models that describe the experiments accurately. The proposed uncertainty characterization approach accounts for parameters related to all measurements, data processing, and finally data interpretation. With the aid of direct numerical simulations, an alternative approach was proposed to derive laminar flame speeds in constant pressure experiments by eliminating the need for using extrapolation equations developed based on simplifying assumptions, which are known to be susceptible to major errors under certain conditions. The propagation of spherical flames under constant volume conditions was investigated through experiments carried out in an entirely spherical chamber and the use of two numerical models. The first involves the solution of the one-dimensional conservation equations of mass, species, and energy while accounting for pressure rise. The second model was developed based on thermodynamics similarly to existing literature, but radiation loss was introduced at the optically thin limit and approximations were made to allow for re-absorption with minimum computational cost. It was shown that neglecting radiation in constant volume experiments could introduce errors as high as 15%. Incorporating the aforementioned techniques, laminar flame speeds were measured and reported with properly quantified uncertainties for flames of syngas for pressures ranging from 3 to 30 atm, and unburned mixture temperatures ranging from 298 to 550 K. Selected measurements were carried out as well for methane and propane flames for pressures ranging from 3 to 7 atm, and unburned mixture temperature of 298 K. The approaches introduced in this study allow for the determination of laminar flame speeds with notably reduced uncertainties under conditions of relevance to engines, which has major implications for the validation of kinetic models of surrogate and real fuels.

1. Introduction

The laminar flame speed, S_u^o, is defined as the propagation speed of a steady, laminar, one-dimensional, planar, stretch-free, and adiabatic flame, hereafter referred to as freely propagating flame. S_u^o is an important fundamental property of a combustible mixture, being a measure of its reactivity, diffusivity, and exothermicity (e.g., [1,2]), an essential validation target for kinetic models, and a key scaling parameter in turbulent combustion.

Given that the freely propagating flame model cannot be reproduced in the laboratory, the accurate measurement of S_u^o has been debated over the years, and data reported from different experimental apparatuses appear to be inconsistent [3]. In addition to being an elusive property for mixtures that result in stable freely propagating flames as is the case for Lewis number $Le > 1$ mixtures, S_u^o does not even have a physical meaning for $Le < 1$ mixtures due to cell development in the absence of stretch. Nevertheless, for both $Le > 1$ and $Le < 1$ mixtures, S_u^o could be viewed as a "concept property" against which kinetic models are validated and/or optimized. There is extensive literature on the topic of laminar flame propagation and the interested reader can consult a number of review articles (e.g., [4–10]).

The first measurements of flame propagation speeds were carried out in 1867 with the experiment of Bunsen [11]. Since then, a larger number of data have been reported in the literature derived from Bunsen flames (e.g., [12–14]), Spherically Expanding Flames (SEF) under constant pressure (e.g., [15–19]) and volume (e.g., [20–26]) conditions, Counter-Flow Flames (CFF) (e.g., [27–29]), and recently the heat flux method (e.g., [30–32]).

---

* Corresponding author. Fax: +1 213 740 8071.
E-mail address: egolfopo@usc.edu (F.N. Egolfopoulos).

http://dx.doi.org/10.1016/j.combustflame.2015.10.003
0010-2180/

Please cite this article as: C. Xiouris et al., Laminar flame speeds under engine-relevant conditions: Uncertainty quantification and minimization in spherically expanding flame experiments, Combustion and Flame (2015), http://dx.doi.org/10.1016/j.combustflame.2015.10.003

A survey of nearly 120 papers published in major combustion journals on the experimental determination of S_u^o, reveals that 65% of the measurements have been carried out at $P = 1$ atm, while only 8% for $P < 1$ atm and 27% for $P > 1$ atm. It is noted also, that the majority of the published S_u^o data, regardless of pressure, correspond to unburned mixture temperatures, T_u, that are either ambient or slightly elevated. Furthermore, the number of flame propagation studies for gaseous fuels is notably higher than those corresponding to liquid fuels.

With few exceptions, S_u^o data are scarce for conditions encountered in piston and jet engines, that is for liquid fuel flames at $P = 20$–50 atm and $T_u = 700$–800 K, given that measurements can be rather challenging and highly uncertain.

Steady-state burner-type laminar flame experiments can be carried out up to $P \approx 10$ atm or so to keep the Reynolds number below its transition value, while experiments at notably higher pressures can be carried out only using SEFs [10,33]. Furthermore, at high pressures S_u^o is the only measurable flame quantity, given that flame structures cannot be resolved due to the decreased flame thickness especially for premixed flames [10,33]. It is also of interest to note that the sensitivity of S_u^o to kinetics is similar to that of extinction strain rate, K_{ext}, of premixed flames as well as non-premixed flames [29,34].

Achieving T_u up to 700–800 K for liquid fuels remains a challenge as well. In order for liquid fuels to exist in the vapor phase at engine-like pressures, the required T_u must be high enough and could result in fuel decomposition both in burner type steady state and static experiments. The vast majority of the flame data reported in the literature during the last 10 years or so for liquid fuels have been measured at $T_u < 500$ K to avoid decomposition in CFFs (e.g., [29,35]) and SEFs (e.g., [36]).

Burner-type experiments such as Bunsen, counterflow, and burner-stabilized flames (e.g., [13,29,31]) are operating under steady state conditions. On the other hand, in order for the reactants to reach a quiescent state in static SEF experiments, several minutes are required upon the completion of the reactant filling process. T_u higher than 500 K in constant pressure SEF experiments could result in fuel decomposition within the several minutes period between filling the chamber and ignition. In addition, high T_u could reduce the effectiveness of the sealing materials and compromise the overall integrity of the apparatus. Thus, in constant pressure SEF experiments (e.g., [16,18,19]) in which measurements are obtained before the compression stage, only moderate T_u values can be tolerated.

The need to measure S_u^o at engine-relevant conditions has been recognized long time ago. Lewis and von Elbe [20] were the first to propose that using the pressure data during the isentropic compression stage in SEF experiments the flame propagation speed could be computed by invoking a number of assumptions and a detailed thermodynamic analysis. This proposition was a pioneering one as during the compression stage notably high pressures and T_u could be achieved within 20 ms or less, a time that is short enough to result in any measurable fuel decomposition and/or to compromise the integrity of the chamber. Bradley and Mitcheson [22] and subsequently Metghalchi and Keck [23,24] adopted the approach of Lewis and von Elbe [20] and developed also thermodynamic models that allowed for the measurement of S_u^o for flames of gaseous and liquid fuels.

While the approach of Lewis and von Elbe [20] was a meritorious one, concerns have been raised about the potential formation of cells that could be unaccounted for in cases that optical access was not possible as well as about potential stretch effects. Metghalchi and co-workers [25,26] resolved the issue of cell formation, by performing measurements first in a cylindrical chamber with optical access and identify thus reactant compositions for which thermal-diffusive and/or hydrodynamic instabilities do not develop during the compression stage when the flame radius is large and the stretch is small. Then, identical initial conditions were established in a perfectly spherical chamber for which the assumptions of the thermodynamic model are applicable. Regarding stretch effects, Metghalchi and co-workers [25,26] argued that they should be small at large flame radii and supported this argument by a series of carefully executed experiments.

In constant pressure SEF experiments, the emphasis is on pressure while T_u is kept either at ambient or slightly elevated values as mentioned earlier. While such S_u^o data are valuable for validating kinetic models at high pressures, very important information stemming from the reactant preheating may be missing. It is well established that while pressure favors three-body low activation energy recombination reactions, temperature favors two-body high activation branching reactions and by considering only one of the two effects may reduce the value of validation.

In addition to the limited thermodynamic conditions at which S_u^o is measured, there are also major concerns related to the accuracy and uncertainty characterization of the reported data. It is unfortunate that subtleties associated with S_u^o measurements have not been recognized properly in past and recent studies, resulting thus in the proliferation of data of questionable fidelity. These subtleties can relate to two-dimensional and unquantified heat loss and fluid mechanic effects in the case of the Bunsen flame method, or to extrapolations to zero stretch in the case of CFFs and SEFs. The issue of data accuracy has been addressed in recent studies [37–39], in which the inadequacies of “standard” extrapolation methods used in CFF and SEF experiments were demonstrated by performing Direct Numerical Simulations (DNS) of the experiments and by performing extrapolations of the DNS data using formulas derived from theories (e.g., [40,41]) that invoke simplifying assumptions. It has been shown that in several instances such formulas fail to reproduce the known S_u^o value by as much as 60% [39]. An additional important result of those studies [37–39] is that using theories based on simplifying assumptions to interpret directly measured data and extract thus S_u^o, could diminish the value of the reported data and that instead DNS should be used, as first proposed by Wang et al. [42].

It is also worth mentioning that a rigorous analysis regarding the uncertainty quantification in data obtained from SEFs does not exist currently in the literature. The transient nature of the experiment along with the cost and effort involved in performing each experiment does not allow for extensive repetitions to obtain statistically significant number of data points.

In view of these considerations, the main goal of this investigation was to introduce an alternative approach to measure S_u^o accurately in SEF experiments under both constant pressure and constant volume conditions. This was achieved by: (1) introducing a detailed uncertainty quantification and propagation methodology and identify thus the key factors that affect the reported S_u^o data; and (2) interpreting the directly measured experimental data using numerical models that constitute the closest possible theoretical representations of the experiments, minimizing thus the data uncertainty.

2. Experimental approach

In order to study laminar flame propagation at variable pressures and T_u, two facilities were used, one cylindrical allowing for full optical access and one spherical without optical access to preserve the sphericity of the apparatus.

Figure 1 depicts the schematic of the cylindrical chamber facility. The chamber is constructed from 316-type stainless steel, measures 270 mm in length and 220 mm in diameter, and can operate up to 90 atm post-combustion pressure. It is fitted with 76 mm thick and 152 mm diameter fused quartz windows at both ends, which are sealed to the chamber with heavy duty O-rings. The initial pressure, P_o, cannot exceed 8 atm in order to avoid failure of the quartz windows during the compression stage of the experiment. The chamber is fitted with two opposing stainless steel electrodes that allow for central ignition. An ignition system has been designed to offer

Please cite this article as: C. Xiouris et al., Laminar flame speeds under engine-relevant conditions: Uncertainty quantification and minimization in spherically expanding flame experiments, Combustion and Flame (2015), http://dx.doi.org/10.1016/j.combustflame.2015.10.003