



## Full Length Article

## Laminar flame speeds of lean high-hydrogen syngas at normal and elevated pressures

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## HIGHLIGHTS

- Laminar flame speeds of lean high-hydrogen syngas were measured.
- A broad range of pressure from 1 atm to 10 atm was considered.
- The performances of three syngas mechanisms were examined.
- Good agreement between simulation and experiments was achieved.

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## ABSTRACT

The laminar flame speed is one of the most important combustion properties of a combustible mixture. It is an important target for chemical mechanism validation and development, especially at fuel-lean and high pressure conditions. In this study, the laminar flame speeds of two types of lean high-hydrogen syngas/oxygen/helium mixtures were measured at normal and elevated pressures up to 10 atm using a dual-chambered high pressure combustion facility. Similar to experiments, numerical simulations of outwardly spherical flame propagation were conducted. Three chemical mechanisms for syngas available in the literature were considered in simulation and their performance in terms of predicting the stretched flame speeds, laminar flame speeds and burned Markstein lengths was examined through comparison between experimental and simulation results. It was found that at both normal and elevated pressures, the present experimental results agree well with those predicted by simulations using these three chemical mechanisms. Therefore, these chemical mechanisms for syngas can well predict the laminar flame properties of lean high-hydrogen syngas. Besides, the laminar flame speeds measured in the present work were compared with those measured from the heat flux method and large difference was observed.

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## 1. Introduction

Synthesized gas (syngas) contains different amounts of CO and H<sub>2</sub> as the primary fuel components. Syngas is one of the most promising alternative fuels since it can be produced from a wide variety of sources, such as coal, biomass, and refinery residuals. Recently, syngas has received great attention due to its application in fuel-flexible gas turbine engines. Depending on the gasification sources and procedures, the composition of syngas varies widely. For example, for coal-based syngas, water–gas shift technologies can be used to generate high-hydrogen syngas. With the increase

in the hydrogen component in syngas, the combustion properties changes greatly. Therefore, high-hydrogen syngas has received great attention recently (e.g., [1–4]). Furthermore, lean syngas combustion at high pressure is promising for achieving high efficiency and low emission in gas turbine engines. Consequently, there is a need to understand fundamental combustion properties of lean high-hydrogen syngas at elevated pressures. In this study, the laminar flame speeds of lean high-hydrogen syngas at elevated pressures were investigated experimentally and numerically.

The laminar flame speed,  $S_L$ , is one of the most important properties of a combustible mixture. It determines the burning rate and flame stabilization in engines. Moreover, it is also an important target for validating chemical mechanisms. Therefore, in the literature there are many studies [1–15] on the laminar flame speed of

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syngas. For examples, Prathap et al. [2] studied the influence of carbon dioxide dilution on the laminar flame speed of syngas (50% $H_2$ –50%CO); Zhang et al. [3] studied the laminar flame speed of lean syngas/air mixtures with a broad range of hydrogen content; Sun et al. [5] studied the laminar flame speed of low-hydrogen syngas within a broad range of pressure from 1 atm to 40 atm; McLean et al. [6] measured  $S_L$  for syngas (5% $H_2$ –95%CO and 50% $H_2$ –50%CO) at atmospheric pressure; and Kong and coworkers [4,17] measured the  $S_L$  of syngas at elevated pressures and temperatures. However, most of the above studies focused on laminar flame speeds at atmospheric pressure or for fuel-rich syngas/air mixtures; and there is a scarcity of high-pressure experimental data for fuel-lean mixtures. Therefore, there is a need to investigate the laminar flame speeds of high-hydrogen syngas at elevated pressure and fuel-lean conditions.

Furthermore, substantial disparities in laminar flame speeds of syngas were observed between experimental data and model predictions at high pressures [1,5,7–9]. The difference between experimental and numerical results might be caused by the uncertainty in experimental measurement and/or the inaccuracy of chemical mechanisms. Goswami et al. [7] measured the laminar flame speeds of lean high-hydrogen syngas at elevated pressures using the heat flux method. They found that compared to experimental data, the laminar flame speeds were greatly over-predicted at elevated pressures by different syngas mechanisms [7]. Therefore, they suggested that the kinetic model for syngas needs further improvement. Since the propagating spherical flame method has the advantage in laminar flame speed measurement at high pressure, this method was used here for the same lean high-hydrogen syngas of Goswami et al. [7] at elevated pressures. Moreover, the experimental data were compared with predictions from different syngas mechanisms in the literature [19–23].

The objectives of this study are to measure laminar flame speeds of lean high-hydrogen syngas at elevated pressures up to 10 atm and to examine the performance of different syngas mechanisms in terms of predicting laminar flame speeds. The paper is organized as follows: in Section 2, the experimental and numerical methods are briefly described; then, in Section 3 the experimental and numerical results are presented together with the discussion on the performance of different syngas mechanisms; and finally, the conclusions are summarized in Section 4.

## 2. Experimental and numerical methods

We studied the same lean high-hydrogen syngas/oxygen/helium mixtures of Goswami et al. [7]: the syngas consists of 85 vol.%  $H_2$  and 15 vol.% CO; and the oxidizer consists of  $O_2$  and He (12.5% $O_2$ –87.5%He for  $\phi = 0.5$  and 11% $O_2$ –89%He for  $\phi = 0.6$ ). Only two mixtures for high-hydrogen syngas were considered: mixture #1 with 85% $H_2$ –15%CO/12.5% $O_2$ –87.5%He and  $\phi = 0.5$ ; and mixture #2 with 85% $H_2$ –15%CO/11% $O_2$ –89%He and  $\phi = 0.6$ . We considered the initial temperature of 298 K and a broad range of pressure from 1 atm to 10 atm. Large amount of helium was included in these mixtures so that stable spherical flame propagation can be achieved at elevated pressures [16].

The laminar flame speeds were measured from outwardly propagating spherical flames in a dual-chambered high pressure combustion facility [4,17]. Detailed description of the experimental system and procedure was presented in [4,17] and thereby only a brief description was given here. The reader is referred to Refs. [4,17] for further details. The combustion chamber consists of two concentric cylindrical chambers. Premixed mixtures were prepared inside the inner chamber (whose inner radius is  $R_w = 5$  cm and length is 15.3 cm) using the partial pressure method. The outer chamber was filled with inert gases to match the inner chamber

pressure. When the mixture was centrally spark-ignited, the spherical flame front history,  $R_f = R_f(t)$ , was recorded using high speed schlieren photography. 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,  $S_b^0$ , and Markstein length,  $L_b$ , both relative to burned gas, can be obtained from extrapolation based on the following linear relationship:

$$S_b = S_b^0 - L_b K \quad (1)$$

where  $K = (2/R_f)(dR_f/dt)$  is the stretch rate of outwardly propagating spherical flames. Finally, the laminar flame speed  $S_L$  is calculated from  $S_L = \sigma S_b^0$ , in which  $\sigma$  is the ratio between burned gas density and unburned gas density. It is noted that there are different linear and nonlinear extrapolations as reported in [24,25]. Wu et al. [25] demonstrated a failure of the linear stretch correction for lean hydrogen flames with systematic over prediction up to 60%. In this study, the effective Lewis number of mixtures #1 and #2 is close to unity and the magnitude of burned Markstein length is within 1 mm. Therefore, the nonlinear behavior is not strong [25] and in fact we found the stretched flame speed changes linearly with the stretch rate for the flame radius range considered in this work (see results shown later). Therefore, the linear extrapolation was used here. Besides, the nonlinear extrapolations might induce large uncertainty in laminar flame speed measurement [26].

The uncertainties of experimental data may come from several sources [34] such as ignition, flame instability, radiation and extrapolation. In the present work, these sources bring little uncertainty for mixtures #1 and #2 and the main source are the uncertainty in the experimental uncertainty ( $\delta_{S_L}$ ) and equivalence ratio ( $\phi$ ). The method of analyzing experimental uncertainty for the  $S_L$  measurement was proposed by Moffat [39], and  $\delta_{S_L}$  can be estimated by the following equation:

$$\delta_{S_L} = \sqrt{(B_{S_L})^2 + [t_{1-\alpha/2}(\nu)\sigma_{S_L}]^2} \quad (2)$$

where  $B_{S_L}$  is the total bias uncertainty and in this study  $B_{S_L}$  is estimated to be about  $\pm 0.9$  cm/s, because  $S_L$  was determined by the linear extrapolation.  $t_{1-\alpha/2}$  is the student  $t$  value at 95% confidence interval and  $\nu$  is the degree of freedom, in present experiments  $\nu$  is estimated to be 12–25.  $\sigma_{S_L}$  is the standard deviation of representing  $S_L$  random uncertainties caused by the initial temperature fluctuation and radiation, etc., here  $\sigma_{S_L}$  was estimated to be about 0.6–1.2 cm/s. From Eq. (2),  $\delta_{S_L}$  was estimated to be about  $\pm 1.5$ –2.8 cm/s. The uncertainty in the equivalence ratio was about  $\pm 2\%$ . And our estimation indicated that the overall uncertainty in the laminar flame speed was within  $\pm 5\%$ .

Besides experiments, the outwardly propagating spherical flames for lean high-hydrogen syngas were simulated using the in house code A-SURF [27–29]. A-SURF solves the conservation equations for a multi-component reactive flow using the finite volume method. A-SURF was used in previous studies on ignition and spherical flame propagation (e.g., [30–34]). The reader is referred to [27–29] for details on governing equations, numerical methods and code validation of A-SURF. In all simulations, the spherical chamber radius was  $R_w = 100$  cm and only flame radius between 0.75 cm and 1.25 cm was utilized for data processing. Consequently, the ignition effects [27,35] and compression effects [28,31] were both negligible. At the initial state, the homogeneous mixture was quiescent at 298 K and specified pressure. Zero flow speed and zero gradients of temperature and mass fractions were enforced at both the center and wall boundaries. Flame initiation was achieved by spatial-dependent energy deposition within a given time period and a given ignition kernel size [31]. In order to adequately resolve the moving flame front, a multilevel, dynamically adaptive mesh was employed and the propagating reaction

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