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Experimental and modelling study of the effect of elevated pressure on ethane and propane flames

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HIGHLIGHTS

- The burning velocities of ethane + air and propane + air flames at elevated pressures were measured.
- Comparison of predictions of 3 mechanisms with the experimental data showed mixed agreement.
- The pressure dependence of the burning velocity was interpreted using empiric power law.
- A sensitivity analysis of the power exponent, beta, of the pressure dependence was performed.

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ABSTRACT

Laminar burning velocities, S_L, of ethane + air and propane + air flames within an equivalence ratio range between 0.8 and 1.3 were determined at atmospheric and elevated pressures up to 4 atm. Measurements were performed in non-stretched flames, stabilized on a perforated plate burner at adiabatic conditions, created using the heat flux method. Initial unburnt gas temperature was 298 K. These new experimental results were compared with available literature data and predictions using three kinetic schemes: USC Mech II, San Diego mechanism and Aramco Mech 1.3. The models behave differently in reproducing S_L of ethane and propane flames with closer agreement between Aramco Mech 1.3 and the present measurements. The pressure dependence of the laminar burning velocities was analysed using the expression $S_L = S_{L0}(P/P_0)^{\beta}$. Large deviations of the derived power exponent, β, were observed for different experimental datasets and between model predictions and the measurements. To elucidate these differences in the performance of the three mechanisms, sensitivity analyses of the burning velocity and of the power exponent β were performed. It was demonstrated that the power exponent β may serve as an independent target for model validation and improvement. When comparing β coefficients derived from the present and previous measurements of S_L in methane, ethane, propane and n-pentane flames using the heat flux method, important similarities were found at lean conditions with large disparity in rich mixtures. Neither experiments nor modelling support the linear dependence of the power exponent β with equivalence ratio for flames of alkanes.

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1. Introduction

Many practical combustion applications such as engines and gas turbines, operate at elevated pressures often 10–30 times higher than atmospheric pressure. Design and optimisation of these devices then requires accurate knowledge of the laminar burning velocity of many conventional fuels and their components at high pressures. Variation of the laminar burning velocity, S_L, with pressure can be interpreted using different empirical correlations outlined, for the case of methane, previously [1]. The most popular correlation describing this effect is

$$S_L = S_{L0}(P/P_0)^{\beta}, \quad (1)$$

where S_{L0} is the burning velocity at reference conditions (usually at 1 atm), and P_0 is the reference pressure. This power-law Eq. (1) is used for about 100 years and has its rationale in early theories of flame propagation. Experimental results accumulated for various hydrocarbon fuels indicated that the power exponent β (sometimes also called baric coefficient) is not a constant for a given fuel and varies with equivalence ratio, initial temperature of the mixture

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and could be different for different pressure ranges. However, the temperature dependence of the power exponent β is often neglected or averaged. The burning velocity of hydrocarbons monotonically decreases with pressure, and β coefficients are almost constant above atmospheric pressure for the same mixture composition, see e.g. [2]. Therefore, the functional dependence of the power exponent β on equivalence ratio, ϕ, is of key importance for proper simulation of high-pressure flames.

It is now well established that homologous hydrocarbons, e.g. normal alkanes, have very similar burning velocities over a wide range of equivalence ratios; other saturated hydrocarbons and alcohols also behave similarly at least for lean mixtures [3]. Hence the suggestion of Metghalchi and Keck [4] in 1982 that β coefficients for several different fuels (including methanol, propane, iso-octane and indolene) can be described by a single dependence

$$\beta = -0.16 + 0.22(\phi - 1) \quad (2)$$

was generally accepted in many applied studies, for example in GT-SUITE software [5], which is one of the leading engine and vehicle simulation tools. Although second-order polynomials were found in a better agreement with available experimental data (for instance for methane [1]), contemporary studies of gasolines and primary reference fuels are still often interpreted by linear functions close to Eq. (2), e.g. [6,7].

To understand whether the effect of pressure on the burning velocity can be generalized, it is vital to investigate and compare experimental and modelling data for homologous hydrocarbons. A number of studies of ethane (C_2H_6) and propane (C_3H_8) flames at atmospheric pressure are available in the literature but scarce at pressures above atmospheric. The primary goal of the present study, therefore, was to investigate the pressure dependence of the laminar burning velocity of ethane and propane flames using the heat flux method. Burning velocities are compared with available literature data and interpreted using Eq. (1). Moreover, experimental results are used to validate the performance of three widely used kinetic models.

2. Experiments

The heat flux method was demonstrated to be suitable for measuring laminar burning velocities at elevated pressures, currently up to 10 atm [1,8–10]. Yet, it has its own limitations related to the formation of cellular flames due to the absence of stretch and increased flame instability at higher pressures especially in rich flames of ethane and propane. Cell formation can easily be detected thanks to optical windows in the high-pressure chamber, and the cell size was always bigger than perforation holes of the burner plate [8]. Consequently, present measurements were mostly limited to 4 atm. Initial temperature of all mixtures studied was 298 K. The high pressure facility employed in the present study and equipped with a gas flow control board, the heat flux system, the high pressure cell, heat exchanger, condenser and exhaust line is fully described by Goswami et al. [9]. Detailed analysis of the heat flux method and typical data processing procedures can be found elsewhere [1,8,9,11].

3. Modelling details

The in-house code CHEM1D [12] was used for modelling one-dimensional freely propagating flames in order to determine the laminar burning velocity and to perform sensitivity analysis. CHEM1D solves a set of equations describing the conservation of mass, momentum, energy and chemical components for chemically reacting flows. It uses an exponential finite-volume discretization in space, and non-linear differential equations are solved with a fully implicit, modified Newton method along with a complex transport model. An adaptive gridding procedure is also implemented to increase the resolution in the flame front by placing almost 80% of the grid points in the area with the largest gradients. The modelling was performed at 1, 2, 3, and 4 atm covering equivalence ratios from 0.7 to 1.4.

Three chemical reaction mechanisms were tested in the present work. The USC Mech II [13] was extensively validated for many fuels including studies relevant to propane flames [14–16]. The San Diego mechanism [17] has been developed through many versions; the latest was selected in the present work. Recent Aramco Mech 1.3 [18] was not specifically validated for propane combustion; it was tentatively tested for both fuels in the present study with encouraging results discussed in the following.

4. Results and discussion

4.1. Ethane flames

The laminar burning velocities of ethane + air flames determined in the present study with associated experimental uncertainties can be seen in Fig. 1 and summarized in Table 1. The range of equivalence ratios covered varies from $\phi = 0.8$ to $\phi = 1.3$ if the flames were stable. Available literature data at elevated pressures are also included in Fig. 1. Hassan et al. [19] obtained laminar burning velocities from spherically expanding flames using linear stretch correction in the range 0.5–4 atm. Jomaas et al. [20] similarly studied spherical flames using linear stretch correction, yet employing a dual-chamber design to mitigate pressure rise, and reported S_L at 1, 2 and 5 atm. From the numerous studies at 1 atm only results of Bosschaart and de Goey [21] are depicted in Fig. 1 to avoid overcrowding of the figure. It was earlier demonstrated [22] that measurements of the burning velocity of ethane + air flames performed using the heat flux method in different labs at atmospheric pressure [21–23] consistently agree within overlapping uncertainties, which is corroborated in the present study.

The present results are in satisfactory agreement with the data of Jomaas et al. [20] at 1 and 2 atm. The significant difference with the measurements of Hassan et al. is difficult to explain even taking into account the rather high uncertainty of S_L evaluated to be about ±9% [19]. Various sources may contribute to the experimental uncertainties in spherical flames, and the difference between datasets may reach 20% even for thoroughly investigated methane flames [24].

Three models tested in the present work behave differently for ethane flames as seen in Fig. 1. The USC Mech II [13] predicts higher burning velocities compared to the two other models and results are closer to the measurements of Hassan et al. [19]. The San Diego mechanism [17] agrees quite well with the USC Mech II in lean mixtures at all pressures; the situation is opposite for the Aramco Mech 1.3 [18], which closely approaches the USC Mech II predictions in rich mixtures.

The measurements and modelling results depicted in Fig. 1 were interpreted using Eq. (1) to derive the power exponents β and to analyse the data consistency over the range of pressures covered. In the literature, only three studies report β coefficients for ethane + air flames. Hill and Hung [2] investigated stoichiometric mixtures of methane with ethane and propane additives in the range of 1–8 atm and obtained $\beta = -0.121$ for pure ethane. In similar experiments Mitu et al. [25,26] processed pressure – time records obtained in a closed vessel explosion of ethane + air with variable initial composition, temperature and pressure in the range from 0.3 to 1.3 atm. The influence of stretch on S_L was ignored and possible flame cellularity was not controlled. Two methods of the data processing [25,26] yielded inconsistent β coefficients different

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