



Full Length Article

Laminar flame properties of C1-C3 alkanes/hydrogen blends at gas engine conditions

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ABSTRACT

The use of fuel blending is encouraged in order to achieve more flexibility in gas engines. In order to design such engines effectively, relevant information about the laminar flame speeds and laminar flame thickness are necessary. Hydrodynamic and thermo-diffusive instabilities at gas engine conditions prevent the acquisition of reliable data experimentally. One-dimensional numerical simulations with detailed chemistry can be a solution. A huge database of laminar flame speeds is generated covering a broad range of gas engine applications, pressure (p) 0.1–20 MPa, fresh gas temperature (T_u) 300–1100 K, air-fuel equivalence ratio (λ) 0.9–2.5, methane 100–60 vol%, ethane 0–40 vol%, propane 0–40 vol%, hydrogen 0–30 vol% and exhaust gas recirculation (EGR) 0–30 m%. The detailed reaction mechanisms GRI 3.0 and AramcoMech 1.3 are used for the generation of flame speed data for the mentioned conditions. A laminar flame speed correlation for 100% hydrogen extending up to elevated pressure and temperature conditions is developed. A blending law based on Le Chatelier's rule is investigated. It is observed that the HC-ratio has a very determining effect for the laminar flame properties of different C1-C3 alkane blends. Based on this observation, it was possible to derive a very efficient correlation for both laminar flame speed and laminar flame thickness for the group of natural gas blends with methane, ethane, propane and hydrogen, and as well as including relevant EGR, which corresponds within 7% accuracy to the calculated database of about 73,000 points. The developed laminar flame speed correlation is incorporated in an engine process simulation code. It is validated with the measured in-cylinder pressure traces from the single cylinder research engine experiments for different gas blends and EGR ratios.

1. Introduction

Gas engines are gaining increased interest because of economical advantages and reduced emissions. Natural gas allows CO₂ emission reduction in the range of 20% compared to conventional fuels like gasoline and diesel due to the lower C/H ratio. Furthermore, gas engines operate without soot and for lean operation conditions with relatively low NO_x emissions. The main constituent of natural gas is methane, with small amounts of heavier hydrocarbons, mainly based on C2-C4. This fraction can significantly vary depending on the source of natural gas up to 18 vol% [1]. The influence of these compounds has a significant effect on the reactivity of natural gas [2]. Further, processes such as gasification of coal or biomass can produce fuels with high hydrogen content and other components up to 38 vol% that are more reactive than methane [3].

Apart from the availability of natural gas surrogate mixtures, blending of natural gas with reactive gases such as ethane or hydrogen is an attractive option to the gas turbine and engine industry. Since it

can extend the flammability limits and can increase the flame speeds at extremely fuel lean conditions [1,4]. Further, the addition of hydrogen reduces pollutant emissions [5,6]. Natural gas blending with higher hydrocarbons such as ethane and propane as well as hydrogen can be an interesting alternative. Furthermore, the use of these mixtures has been subject to a very large number of studies in relation to engine applications but also in relation to the gas supply industry where there have been a number of significant studies recently [7,8].

Heavy duty gas engines in particular operate on fuel lean conditions with diluted mixtures. This can be achieved either with excess air, leading to a “lean burning” mode, or with exhaust gas recirculation (EGR), being sometimes called as “ $\lambda = 1 + \text{EGR}$ ” engine [9,10]. Both dilution methods reduce the combustion temperatures which lead to lower NO_x emissions and to lower heat losses to the walls, hence, the efficiency of the gas engine is increased.

However, the dilution is limited to a certain extent as the reactivity and laminar flame speed decreases, which can reduce the burn out, it can lead to combustion instabilities and to flame quenching. Near this

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limit, the unburned hydrocarbon emission (UHC) increases and the engine efficiency decreases.

Laminar flame speed S_L is fundamental not only for the reaction progress but also for the design of any combusting system, as it is determinant for combustion phenomenon such as flame stabilization, quenching, turbulent flame structure and plays a vital role in several aspects of combustion processes in spark ignition engines and/or gas turbines [10,11]. Ranzi et al. [12] reviewed experimental data of laminar flame speeds of CH_4 /air mixtures at different temperature and pressure conditions available in literature and emphasized on scatter in the measurements. Commonly used experimental methods for the measurement of laminar flame speeds are, such as the spherical flames in constant volume or constant pressure chambers [13,14], counter flow flames [15] and flat flame adiabatic burner (heat-flux method) [2,16].

Laminar flame speeds of pure hydrogen have been measured by several groups at atmospheric conditions of 1 atm and 298 K for a broad range of air-fuel equivalence ratios [17–19]. Kerjci et al. [20] conducted closed vessel experiments for pure hydrogen at 1 atm for higher temperatures up to 443 K. However, measurements for unstretched S_L of pure hydrogen at elevated pressures are extremely difficult to achieve [21]. This is due to the higher sensitivity of hydrogen to thermo-diffusive and hydrodynamic instabilities leading to unstable cellular flame structures. The same problem is relevant for high hydrogen blended fuels [22].

Yu et al. [23] published measured laminar flame speed data of CH_4 blended with H_2 up to 50 vol% using the counterflow method. Several research groups have published measurement data of CH_4/H_2 blends [24–26] up to 40 vol% H_2 . Hu et al. [27] conducted CH_4/H_2 blending laminar flame speed experiments using the combustion bomb method. This data was later theoretically investigated by Al-Mughanam et al. [28], where different blending laws were investigated. Dirrenberger et al. [2] published CH_4/H_2 blending laminar flame speeds using the heat flux method. As per the authors knowledge, only Plichta et al. [1] conducted methane/hydrogen blending from 50 to 90 vol% H_2 at elevated pressures up to 5 atm using the combustion vessel method.

Few research groups have published laminar flame speed data for realistic natural gas mixtures [2,3,8,16]. Dirrenberger et al. [2] investigated pure methane, ethane, propane, butane and natural gas surrogate mixtures consisting of different proportions of ethane and propane up to 82 vol% methane. Kochar et al. [16] conducted laminar flame speed experiments for pure methane and binary blends of CH_4/C_2H_6 and CH_4/C_3H_8 at elevated pressures up to 10 atm and 650 K. Nillson et al. [7] measured laminar burning velocities of hydrocarbon blends of relevance to natural gas combustion, with addition of 0, 10, 35 and 50% hydrogen using the heat flux method.

For conditions relevant to gas engines, where the in-cylinder pressures can reach up to 20 MPa and the fresh gas temperatures can be higher than 1000 K, the experimental data is very difficult to obtain due to the effects of flame stretch and instabilities. Instead, detailed one-dimensional numerical simulations can be conducted, including the detailed reaction mechanism as well as the diffusive transport processes inside the reaction zone [10,29,30], to obtain the laminar flame speed database for the gas blends at engine relevant conditions. Ratzke et al. [10] created a tabulated laminar speed database using the GRI 3.0 mechanism [31] for methane at gas engine conditions as a function of four parameters, λ , T_u , p and Y_{EGR} (mass fraction of EGR). Tabulated data, however, leads to very expensive interpolation procedures, especially when the number of parameters increases, as in the situation of fuel blends. This is even more important when calculations within 3D CFD simulations are anticipated [11].

Mathematical correlations for the laminar flame speeds would allow calculations with significantly reduced computational cost. These correlations can be derived from the database obtained from 1D numerical simulations using detailed reaction mechanism appropriate for the engine conditions [22,32,33]. For gas blends, the blending effect has a

non-linear evolution effect on the laminar flame speed. This leads to complicated mathematical correlation equations to capture this behaviour [22].

In the present work, a laminar flame speed correlation is developed as a function of seven parameters: air-fuel equivalence ratio, pressure, temperature, mole fractions of ethane, propane, hydrogen and EGR ratios for gas engine conditions. This 7D matrix is reduced to a 4D matrix, where the gas composition information is incorporated in terms of the hydrogen to carbon ratio (HC-ratio or HC) in a block-structured pattern. This will be explained in the following sections. Complications in the mathematical correlations due to the blending effects, are taken into account, in which the coefficients are calculated in a pre-processing manner. The coefficients in the present work are entirely the functions of mixture composition, i.e., they contain the information regarding the air-fuel equivalence ratio (λ), mole fractions of ethane ($X_{C_2H_6}$), mole fractions of propane ($X_{C_3H_8}$), mole fraction of hydrogen (X_{H_2}) and the exhaust gas recirculation (Y_{EGR}) in the methane mixture. Since most gas engines operate with premixed combustion, hence the composition is already known. This enables the laminar flame speed to be just a 2D function of pressure and temperature for the whole simulation. Even in the case of scavenged prechamber ignition, it is not a concern, since the gas composition variation lasts for just a few crank angle degrees. In addition, an S_L correlation for pure hydrogen is developed for engine conditions as a part of this block-structured approach. Details of this approach is discussed in further sections.

2. Influence of HC-ratio

Warnatz [29] suggested the reactions $\dot{H} + O_2 = \ddot{O} + \dot{OH}$ and $CO + \dot{OH} = CO_2 + \dot{H}$, as the most fundamental reactions for the combustion of any hydrocarbon fuel up to 16 carbon atoms (with the dots indicating the unsaturated free electrons of the radicals). The other major sensible reaction being $\dot{H} + O_2 (+M) = H\ddot{O}_2 (+M)$. Kochar et al. [16] conducted sensitivity analysis for their experiments for pure methane, ethane, propane and the blends 60% $CH_4/40\%$ C_2H_6 and 60% $CH_4/40\%$ C_3H_8 at 298 K and 5 atm. It is seen that the first chain branching reaction is the most important at high temperatures. It shows that the highest sensitivity for the case of pure methane and the sensitivity decreases when moving towards ethane/propane. The CO oxidation reaction is the second most significant reaction, whose promoting effect remains constant for all conditions. It varies more with the stoichiometry than with blending fractions.

However, the most significant finding of the group's sensitivity analysis being that no reactions involving the parent molecules C_2H_6 or C_3H_8 were present. The abstraction and recombination reactions, $CH_4 + \dot{H} = CH_3 + H_2$ and $CH_3 + \dot{H} (+M) = CH_4 (+M)$, being significant reactions involving parent CH_4 molecule for all blends. Metcalfe et al. [34] suggested the importance of C3 and C4 chemistry to describe the kinetics of CH_4 and C_2H_6 , such as the recombination reactions, $\dot{C}H_3 + \dot{C}_2H_5 = C_3H_8$ and $\dot{C}_2H_5 + \dot{C}_2H_5 = nC_4H_{10}$. These reactions are however, significant for fuel rich conditions. It can be concluded from the literature, that for the lean gas engine conditions, it is the small species chemistry that is fundamental for the kinetics of combustion of larger hydrocarbons.

HC-ratio describes the availability of hydrogen atoms and carbon atoms in gas mixture which can be vital to describe its reactivity and is defined as a ratio of the total number of hydrogen atoms to the total number of carbon atoms per mole of a hydrocarbon gas mixture, as shown in Eq. (1).

$$HC = \frac{4 \cdot X_{CH_4} + 6 \cdot X_{C_2H_6} + 8 \cdot X_{C_3H_8}}{1 \cdot X_{CH_4} + 2 \cdot X_{C_2H_6} + 3 \cdot X_{C_3H_8}} \quad (1)$$

For a given hydrocarbon gas mixture, $X_{CH_4} + X_{C_2H_6} + X_{C_3H_8} = 1$. $X_{C_xH_y}$ denotes the mole fraction of the respective hydrocarbon in the gas mixture.

These conclusions can further explain the methane-number MN

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