Short communication

A laminar burning velocity correlation for combustion simulation of hydrogen-enriched ethanol engines

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ABSTRACT

In this paper, a laminar burning velocity correlation was proposed for combustion simulation of hydrogen-enriched ethanol engines. This correlation was developed based on the flame–temperature-based mixing rule. Wide ranges of hydrogen mole fraction, equivalence ratio, unburned gas temperature, pressure, and residual gas mass fraction were simultaneously considered in the correlation to cover the burning conditions encountered in the spark-ignited (SI) engine combustion. Computational fluid dynamics (CFD) calculations were performed with the implementation of this correlation. This correlation was confirmed to be suitable for engine simulation since the CFD model could well capture the combustion behavior in hydrogen-enriched ethanol engines.

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1. Introduction

In recent years, the diminishing fossil fuel reserves have inspired efforts on exploring alternative fuels for internal combustion engines. Ethanol is considered as a promising option since it can be derived from various renewable resources [1]. However, because of the high latent heat of ethanol, the pure ethanol-fueled engines always suffer deteriorated performance at cold start and idle conditions [2], which is a main barrier to its commercialization. Comparatively, due to the gaseous state, low ignition energy and extremely high flame speed of hydrogen, the hydrogen enrichment has been found to be effective on promoting the in-cylinder charge homogeneity and improving the turbulent combustion [3,4]. Moreover, as hydrogen can be generated from on-board reforming of ethanol, the problems associated with hydrogen production and storage can be solved with little modification for an ethanol engine-powered vehicle [5]. Thereby, the hydrogen-enriched ethanol engine seems an effective and practical approach for future SI engines.

Laminar burning velocity is an intrinsic characteristic of combustible mixtures, which not only determines the engine combustion phenomena but also provides fundamental data for calculating in-cylinder flame propagation in turbulent combustion models. Li et al. [6] experimentally measured the laminar burning velocity of hydrogen–ethanol–air mixtures and observed that the hydrogen

addition exponentially enhances the ethanol laminar burning velocity. More recently, the chemical kinetic calculations conducted by Al-Hamamre and Yamin [7] demonstrated that the enhanced laminar burning velocity is caused by the stimulated H, O, and OH radicals in the flame front after the hydrogen enrichment.

Although previous investigations have reported the laminar burning velocity of hydrogen–ethanol–air mixtures under some specified burning conditions, however, there is still no published data covering the engine-relevant burning conditions. This blocks the combustion modeling for hydrogen-enriched ethanol engines. Thus, a laminar burning velocity correlation of hydrogen–ethanol blends is developed for engine simulation in this paper. Its suitability for engine simulation is examined through CFD calculation and experimental test.

2. Description of the approach

2.1. Evaluation of laminar burning velocity models for hydrogen–ethanol blends

Up to now, there are five models available for estimating the laminar burning velocity of binary fuel mixtures under varying burning conditions, including the Le Chatelier's Rule-like formula suggested by Di Sarli and Di Benedetto [8], the flame–temperature-based mixing rule proposed by Hirasawa et al. [9] and Ji and Egolfopoulos [10], and the mixing rules based on mole, mass, and energy fractions of the fuel component mentioned by Sileghem et al. [11].

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Fig. 1 compares the experimentally measured laminar burning velocities of hydrogen–ethanol blends reported in Ref. [6] with those estimated by these models under an unburned gas temperature of 383 K, a pressure of 0.1 MPa and stoichiometric conditions. The experimental data of neat hydrogen and ethanol are used as inputs in these models. It can be observed that the flame–temperature-based mixing rule reproduces the experimental results with satisfying accuracy. This can be attributed to the following facts. As it is suggested by Ji et al. [10], the flame–temperature-based mixing rule is valid for fuel mixtures whose laminar burning velocity is mostly sensitive to the flame temperature through its influence on the main branching reaction $H + O_2 \rightarrow OH + O$. As a consequence, this model can be applied when the two neat fuel components interact predominantly through reactions with generic flame radical species such as H, O, and OH. Meanwhile, the hydrogen enrichment is also observed to accelerate the laminar flame propagation of the ethanol–air mixture through stimulating the H, O, and OH radicals in the flame front [7]. This means the sensitivity of ethanol laminar burning velocity on the branching reaction $H + O_2 \rightarrow OH + O$ is more pronounced after the hydrogen enrichment. Thus, although the effects of pressure and hydrogen diffusivity have been neglected, the flame–temperature-based mixing rule tends to be predictive for binary fuel mixtures of hydrogen and ethanol with satisfying accuracy.

2.2. Calculation step and laminar burning velocity correlation

Based on the above analysis, the flame–temperature-based mixing rule is selected to compute laminar burning velocities of hydrogen–ethanol blends for varying burning conditions and hydrogen enrichment levels. According to this mixing rule, the laminar burning velocity can be computed by Eq. (1):

$$S_{L,hydrogen+ethanol} = \exp\left[\tau_{hydrogen} \cdot \ln S_{L,hydrogen} + \tau_{ethanol} \cdot \ln S_{L,ethanol}\right] \quad (1)$$

where the laminar burning velocities of hydrogen–ethanol blends, neat hydrogen, and neat ethanol are symbolized by $S_{L,hydrogen+ethanol}$, $S_{L,hydrogen}$, and $S_{L,ethanol}$, respectively. The $\tau_{hydrogen}$ and $\tau_{ethanol}$ are dimensionless numbers indicating the contributions of hydrogen and ethanol to the adiabatic flame temperature of total fuel, respectively.

During the calculation, $S_{L,hydrogen}$ and $S_{L,ethanol}$ are derived from the correlations reported in Refs. [12,13], respectively. These two

correlations are selected based on the consideration that they are valid at wide range of burning conditions and consequently suitable for engine simulation. $\tau_{hydrogen}$ and $\tau_{ethanol}$ are computed by:

$$\tau_i = \frac{1}{T_{ad,m}} \cdot \left(\frac{X_i \cdot N_i}{N_m} \cdot T_{ad,i}\right) \quad (2)$$

The subscript i indicates hydrogen or ethanol, while subscript m represents binary fuel mixture of hydrogen and ethanol. X is the mole fraction of hydrogen or ethanol in the binary fuel mixture. N and T_{ad} stand for the total number of moles of the combustion products and adiabatic flame temperature, which could be determined through an iterative calculation for species composition and adiabatic heat release [14].

Subsequently, a laminar burning velocity dataset is generated from the above calculation. In this dataset, the hydrogen mole fraction in the total fuel (X_{H2}) varies from 0% to 100% with steps of 5%. The equivalence ratio (Φ) varies from 0.6 to 1.5 with steps of 0.1. The unburned gas temperature (T_u) varies from 400 to 1000 K with steps of 100 K. The pressure (p) varies from 0.1 MPa and then 0.5–5.0 MPa with steps of 0.5 MPa. The residual gas mass fraction (Y_{dil}) varies from 0% to 20% with steps of 5%. This dataset totally contains 80,850 data points, which could cover the burning conditions encountered in SI engines.

Since correlations are more computationally efficient than dataset for engine simulation, a laminar burning velocity correlation is developed based on the dataset, which follows the format proposed by Metghalchi and Keck [15]:

$$S_{L,hydrogen+ethanol}(X_{H2}, \Phi, T_u, p, Y_{dil})$$
$$= S_{L,0} \cdot \left(\frac{T_u}{T_{ref}}\right)^\alpha \cdot \left(\frac{p}{p_{ref}}\right)^\beta (1 - \gamma Y_{dil}) \quad (3)$$

In this correlation, $S_{L,hydrogen+ethanol}$ (cm/s) can be directly deduced according to X_{H2}, Φ, T_u (K), p (MPa), and Y_{dil}. The reference temperature T_{ref} and reference pressure p_{ref} are equal to 400 K and 0.1 MPa, respectively. The parameters $S_{L,0}$, α, β, and γ are determined through Eqs. (4)–(7).

$$S_{L,0} = \left(a_0 + a_1\Phi + a_2\Phi^2 + a_3 X_{H2} + a_4 X_{H2}^2\right)$$
$$\cdot \left[(a_5 + a_6\Phi + a_7\Phi^2) + a_8 \exp(a_9 + a_{10}\Phi + a_{11}\Phi^2 + a_{12}X_{H2} + a_{13}X_{H2}^2)\right] \quad (4)$$

$$\alpha = b_0 + b_1\Phi + b_2\Phi^2 + b_3 X_{H2} + b_4 X_{H2}^2 + b_5\left(\frac{T_u}{T_{ref}}\right) + b_6\left(\frac{T_u}{T_{ref}}\right)^2$$
$$+ b_7\Phi X_{H2} + b_8\Phi\left(\frac{T_u}{T_{ref}}\right) + b_9 X_{H2}\left(\frac{T_u}{T_{ref}}\right) + b_{10}\Phi^2 X_{H2}$$
$$+ b_{11}\Phi X_{H2}^2 + b_{12}\Phi^2 X_{H2}^2 + b_{13}\Phi\left(\frac{T_u}{T_{ref}}\right)^2 + b_{14}X_{H2}\left(\frac{T_u}{T_{ref}}\right)^2 \quad (5)$$

$$\beta = c_0 + c_1\Phi + c_2\Phi^2 + c_3 X_{H2} + c_4 X_{H2}^2 + c_5\Phi X_{H2} + c_6\Phi^2 X_{H2}$$
$$+ c_7\Phi X_{H2}^2 + c_8\Phi^2 X_{H2}^2 \quad (6)$$

$$\gamma = d_0 + d_1\Phi + d_2\Phi^2 + d_3 X_{H2} + d_4 X_{H2}^2 + d_5\Phi X_{H2} + d_6\Phi^2 X_{H2}$$
$$+ d_7\Phi X_{H2}^2 + d_8\Phi^2 X_{H2}^2 \quad (7)$$

Eqs. (4)–(7) totally contain 47 fit coefficients which are determined through the Levenberg–Marquardt method [16]. The values of these fit coefficients are listed in Table 1. Through comparing the values estimated from this correlation with those in the dataset for all the fitted data points (80,850 in total), it is observed that the coefficient of determination R^2 achieves 0.9945, suggesting that this correlation could well reproduce the dataset values.
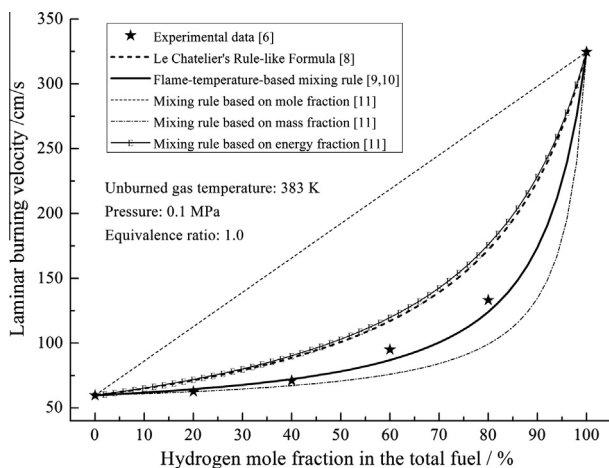

Fig. 1. Comparison of the experimentally measured laminar burning velocities with those estimated using different models under normal burning condition.