

# Numerical Investigation of Laminar Flame Speed of Gasoline - Ethanol/Air Mixtures with Varying Pressure, Temperature and Dilution

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## ABSTRACT

A numerical analysis was performed to study the variation of the laminar burning speed of gasoline-ethanol blend, pressure, temperature and dilution using the one-dimensional premixed flame code CHEMKIN™. A semi-detailed validated chemical kinetic model (142 species and 672 reactions) for a gasoline surrogate fuel was used. The pure components in the surrogate fuel consist of n-heptane, isooctane and toluene. The ethanol mole fraction was varied from 0 to 85 percent, initial pressure from 4 to 8 bar, initial temperature from 300 to 600K, and the EGR dilution from 0 to 32% to represent the in-cylinder conditions of a spark-ignition engine. The laminar flame speed is found to increase with ethanol concentration and temperature but decrease with pressure and dilution. A correlation has been proposed to calculate laminar flame speeds of gasoline-ethanol/air mixtures at different pressures, temperatures, and EGR that can be used in parametric burn rate combustion models for engine simulation.

## INTRODUCTION

The laminar burning speed is an important parameter for premixed combustion calculations. It is useful to predict the pressure rise inside internal combustion engines and the turbulent flame speeds [1-2]. Turbulent flame propagation models are based on the laminar burning speed and turbulence intensity [3]. Laminar burning speeds are also used for determination of ignition delay and wall quench layer thicknesses [4-5]. For a given fuel, the laminar burning speed, amongst other parameters, is a function of the mixture strength and the unburned mixture temperature and pressure. It also depends on the mass fraction of the residual gases in the fresh mixture (EGR).

Several correlations of laminar burning speed for different fuels are available in the literature. These correlations describe the influence of air-fuel ratio, pressure, temperature, and EGR on the laminar burning speed. The experiments upon which the correlations are based are normally conducted in constant volume combustion vessels at several initial pressures and temperatures. For single component fuels such as methanol, ethanol, and isooctane, Gulder [6] proposed a correlation for Laminar Flame Speed [LFS], based on experimental evidence, of the form;

$$S_L = S_{L,0} \left( \frac{T_u}{300} \right)^\alpha \left( \frac{P}{1.013} \right)^\beta \quad (1)$$

Gulder [7] also studied the effect of dilution on LFS for single component fuels like methanol, ethanol, and isooctane and proposed a correlation that was capable of predicting the effect of dilution on LFS.

$$S_L = S_{L,0} \left( \frac{T_u}{298} \right)^\alpha \left( \frac{P}{1.013} \right)^\beta (1 - 2.3x_d) \quad (2)$$

The author argued that the values of  $\alpha$  and  $\beta$  are independent of type of fuel and are functions of equivalence ratio only.

Metagalchi and Keck [8] carried out experiments with methanol, isooctane, and indolene (RMFD-303) in the temperature range of 298 K to 700 K and proposed a correlation to estimate LFS, which is similar to Gulder with the exception of the residual fraction coefficient being 2.1 instead of 2.3. They proposed a correlation of the form;

$$S_L = S_{L,0} \left( \frac{T_u}{298} \right)^\alpha \left( \frac{P}{1.013} \right)^\beta (1 - 2.1x_d) \quad (3)$$

They also observed that the values of  $\alpha$  and  $\beta$  are independent of the type of fuel and proposed the value of  $\alpha$  to be 2.18 and  $\beta$  to be -0.16 for the above mentioned single component fuels.

Annand [9] used the correlation proposed by Metghalchi and Keck for LFS and proposed a correlation for Turbulent Flame Speeds with propane and isooctane.

Rhodes and Keck [10] measured the laminar burning speeds of Retail Motor Fuel Dispenser-303 (RMFD-303) and RMFD-302 (indolene)-air mixtures over a pressure range of 0.4 atm to 12 atm, temperature range of 350K to 550K with  $N_2$  and  $CO_2$  as diluents. They also concluded that  $\alpha$  and  $\beta$  are approximately independent of type of fuel and are functions of equivalence ratio only. Based on their experimental results they proposed a new correlation for LFS of the type;

$$S_L = S_{L,0} \left( \frac{T_u}{298} \right)^\alpha \left( \frac{P}{1.013} \right)^\beta (1 - 2.06x_d^{0.733}) \quad (4)$$

The authors argued that LFS for both the multi-component fuels peak at an equivalence ratio ( $\Phi$ ) of 1.2 and  $\beta$  becomes positive for  $\Phi > 1.4$ . They found both RMFD-303 and RMFD-302 to be similar to automotive gasoline.

Heywood [2] summarized the results of several experimental studies and proposed a correlation;

$$S_L = S_{L,0} \left( \frac{T_u}{298} \right)^\alpha \left( \frac{P}{1.013} \right)^\beta (1 - 2.06x_d^{0.77}) \quad (5)$$

Heywood also reasoned that  $S_{L,0}$ ,  $\alpha$ , and  $\beta$  were constants for a given fuel, equivalence ratio and burned gas diluents fraction. For propane, isooctane and methanol, these constants can be represented by

$$S_{L,0} = B_m + B_\phi (\phi - \phi_m)^2 \quad (6)$$

$$\alpha = 2.18 - 0.8(\phi - 1) \quad (7)$$

$$\beta = -0.16 + 0.22(\phi - 1) \quad (8)$$

For gasoline (a reference gasoline with average molecular weight of 107 and H/C ratio of 1.69);

$$\alpha_g = 2.4 - 0.271\phi^{3.51} \quad (9)$$

$$\beta_g = -0.357 + 0.14\phi^{2.77} \quad (10)$$

Where  $B_m$ ,  $B_\phi$  and  $\Phi_m$  are constants that differ for different fuels. For gasoline these values are 0.305m/s, -0.549m/s, and 1.21 respectively.

Takashi and Kimitoshi [11] studied the LFS of fuels like isooctane, n-heptane and ethanol experimentally for a range of equivalence ratios from 0.7 to 1.5 and tabulated values of flame speed for the above mentioned fuels.

Computational study of combustion in engines is an essential complementary tool to engine experiments. Especially since computation allows testing of a large number of variables without modifying existing plants. Computations can predict performance at any scale in a relatively short period of time and are particularly useful in simulating conditions during which it is not possible to take detailed measurements. To study the combustion process computationally in HCCI and SI engines, chemical kinetic models are needed to represent the combustion of the fuels. In recent years, detailed chemical kinetic models have been developed to fully describe the fundamental chemical processes involved in single component fuel oxidation. For example, Curran et al. [12-13] developed comprehensive mechanisms to study the oxidation of n-heptane and isooctane having 560 species and 2539 reactions, and 857 species and 3606 reactions, respectively. The mechanisms were validated by comparing computed results with experimental data over a wide range of temperatures and pressures and reasonable agreement was reported.

Battin-Leclerc et al. [14] developed a software package "EXGAS" to automatically generate detailed kinetic models for gas-phase oxidation and combustion of normal and branched alkanes, including n-butane, n-octane, n-decane, n-hexadecane, n-heptane, and isooctane and Primary Reference Fuel (PRF) mixtures.

Conventional automotive engines use gasoline or diesel as fuel, which are multi-component fuels. Reaction mechanisms that consist of several hundred species and several thousand reactions, like that of gasoline are currently too complex to use in a detailed chemical kinetic mechanism. Composition of these fuels varies depending on the source of the fuel and its production history. Gasoline fuels exhibit tremendous complexities due to this range of hydrocarbon constituents, and it is practically impossible to include every individual

component in modeling the mixture preparation and subsequent combustion processes. Therefore, it is desirable to use a chemical reaction mechanism that retains the essential features of the fuel chemistry predicted by the complete mechanisms, but with much improved computational efficiency in terms of memory usage and computational time. It is also desirable to limit the chemical and physical complexity of the fuel to generate insight and understanding into the underlying fundamental processes. For the above mentioned reasons a surrogate gasoline fuel with a finite number of compounds and a standard composition that closely matches practical fuels is employed for studying the flame speeds and the auto-ignition chemistry. According to Machrafi-Cavadias [15] and Andrae - Head [16] it is widely accepted that the oxidation processes of n-heptane, isooctane, and toluene represent the ignition and combustion characteristics of gasoline fuels well, hence the effect of composition changes of multi-component fuels like gasoline can, as a first approximation, be simulated using blends of these three pure hydrocarbons. Table 1 gives the composition (liquid volume %) of gasoline surrogate fuels defined by Machrafi-Cavadias and Andrae-Head.

**Table 1. Composition (liquid volume %) of gasoline surrogate.**

| Name              | n-Heptane | Isooctane | Toluene |
|-------------------|-----------|-----------|---------|
| Andrae-Head       | 17        | 63        | 20      |
| Machrafi-cavadias | 11        | 59        | 30      |

Machrafi-Cavadias investigated the autoignition of gasoline using the above mentioned surrogate and validated it with reasonable accuracy using experimental results. Andrae-Head used the surrogate gasoline for modeling HCCI experiment

Dagout-Togbe [17] also used a reduced mechanism with ethanol, isooctane, toluene, and 1-hexene to study the oxidation kinetics of gasoline and reported good agreement between experimental results and the computations using the reduced mechanism.

Katta-Roquemore [18] used a Jet-propellant JP-8 surrogate mixture to predict flame extinguishment. Their results compared favorably with results obtained using their own mathematical model, UNICORN. Andrae et al. [19] used a semi-detailed mechanism containing 137 species and 633 reactions to obtain laminar burning speeds of benzene/air and toluene/air mixtures and a real gasoline air mixture. They reported the results to be in good agreement with the experimental results after some revision of the high temperature chemistry. They also reported their model was sensitive to molecular structure effects on laminar flame speeds. Egolfopoulos et al. [20] proposed a new complete mechanism, capable of closely predicting the experimental

LFS of ethanol, methane, methanol and all the C2 hydrocarbons. The mechanism was validated against experimental data on the species and temperature profiles in flow reactors and on ignition delay times in shock tubes.

Davis et al. [21] experimentally studied the laminar flame speeds and oxidation kinetics of benzene-air and toluene- air flames at standard conditions. The authors found the experimental results to be substantially higher than the computed values. The mechanisms used for computation were Emdee-Brezinsky-Glassman (EBG) [22] and Lindstedt and Skevis (LS) [23].

Habik et al. [24] developed a reduced reaction mechanism for high hydrocarbon fuels including gasoline, kerosene (JP-8), and n-hexadecane over a temperature range of 300 K to 700 K, a pressure range of 0.11 atm to 10 atm, and an equivalence ratio ( $\Phi$ ) range of 0.5-1.5. The mechanisms developed showed good agreement with experimental results at lean to near stoichiometric conditions.

## OBJECTIVE

Most of the above mentioned researchers presented their own reduced mechanisms for each individual fuel while comparing them with the experimental results of ignition delay and oxidation kinetics. However, there were very few researchers who studied the LFS of real gasoline experimentally or computationally. To address this need, the present study involves computation of LFS of various gasoline-ethanol blends using the commercial code CHEMKIN™.

The objectives of the present study are to compute the laminar burning speeds of gasoline-ethanol blends using a reduced chemical kinetics model to investigate the effects of ethanol concentration, pressure, temperature, and dilution on the laminar burning speeds. A correlation is developed that is capable of predicting the effects of the different variables on LFS.

To achieve the above mentioned objectives, numerical simulations were conducted using a semi-detailed chemical kinetic model (142 species and 672 reactions) for gasoline surrogate fuels [16]. This mechanism, here after referred to as the Andrae-Head mechanism, was chosen because of its ability to describe the fuel consumption rates as well as the important intermediate species profiles in HCCI experiments. The mechanism consisted of a detail description of toluene oxidation and skeletal mechanisms for isooctane and n-heptane. The toluene mechanism involved a detailed benzene sub-mechanism consisting of an oxidation subset for C1-C6 hydrocarbons, together with a small subset for reactions involving NO. The mechanism also includes ethanol, frequently used as a blend component, which made this mechanism preferable over other available mechanisms.

Gulder [6] explained the importance of investigating the effects of ethanol addition by showing the behavior of the spark timing in an engine fuelled with ethanol. According to the author, spark ignition engines fuelled with ethanol require less advanced spark timing as compared to those fuelled by gasoline. However, according to Takashi et al. [11] gasoline-alcohol blends require more advanced spark timing for maximum torque output than for those using gasoline and alcohols independently. The authors argued that the addition of ethanol to fuels like n-heptane and isooctane-air flames stabilizes the flames in the fuel rich regions. Yeliana et al. [25] also studied the effect of ethanol addition to gasoline and found that with an increase in ethanol concentration the burn duration reduces indicating a faster burn rate. They also found that with increase in ethanol concentration the cycle to cycle variation in engine operation reduces allowing a wider range of operation with lean mixtures and high dilution.

## RESULTS AND DISCUSSION

### Model Validation

The experimental results provided by Egolfopoulos et al. [20] were used to validate the Andrae-Head mechanism. The reported maximum experimental uncertainty was  $\pm 10\%$ . Figure 1 shows the comparison of experimental and computed LFS for pure ethanol.

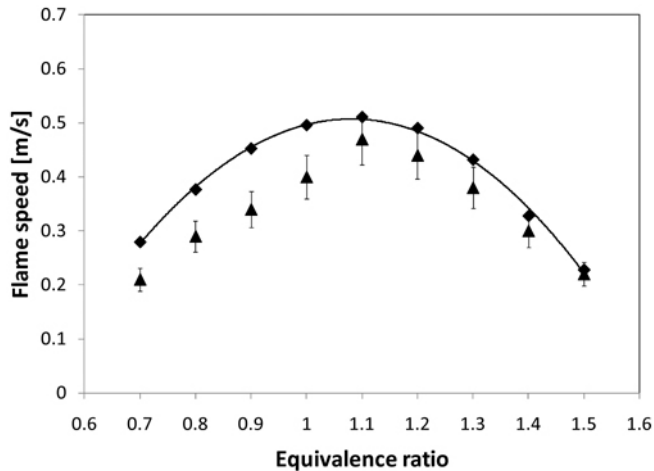


**Figure 1.** Comparison of experimental ( $\blacktriangle$ ) [20] and computed ( $\text{—}\blacklozenge\text{—}$ ) laminar burning velocities for ethanol/ air mixtures at 1 atm and 298 K, the reported maximum uncertainty of the experiments is  $\pm 10\%$ .

In Figure 1 the burning velocities are over predicted by the model at lean to stoichiometric fuel- air ratios, suggesting the ethanol sub-mechanism in Andrae-Head mechanism to be more reactive.

Figure 2 gives the comparison of experimental [26] and computed LFS for 80% isooctane – 20 % ethanol / air

mixture. The burning velocities are under predicted by the model. The difference between the model and the experiment was greater at lean to stoichiometric fuel/ air ratios; however the difference was approximately 10 % at stoichiometric to rich fuel/air ratios.

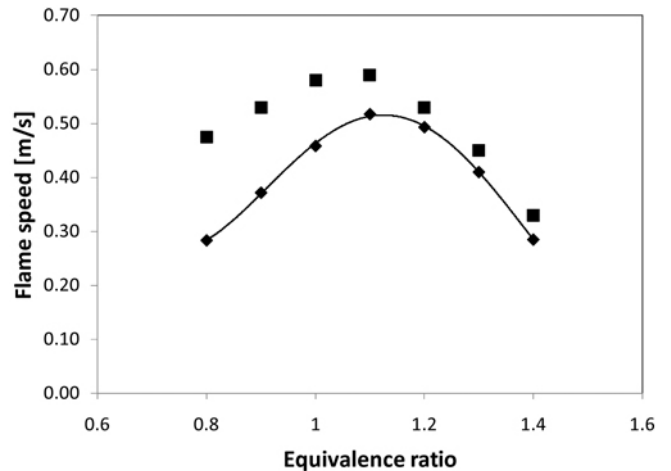


**Figure 2.** Comparison of experimental ( $\blacksquare$ ) [26] and computed ( $\text{—}\blacklozenge\text{—}$ ) laminar burning velocities for 80% iso-Octane plus 20% ethanol/ air mixtures at 350K and 1 atm.

Figure 3 shows the comparison of LFS of n-heptane at 325 K and 100 kPa using the complete mechanism from LLNL [12] and the Andrae-Head mechanism. The difference between the results at  $\Phi=1$  is approximately 4%.

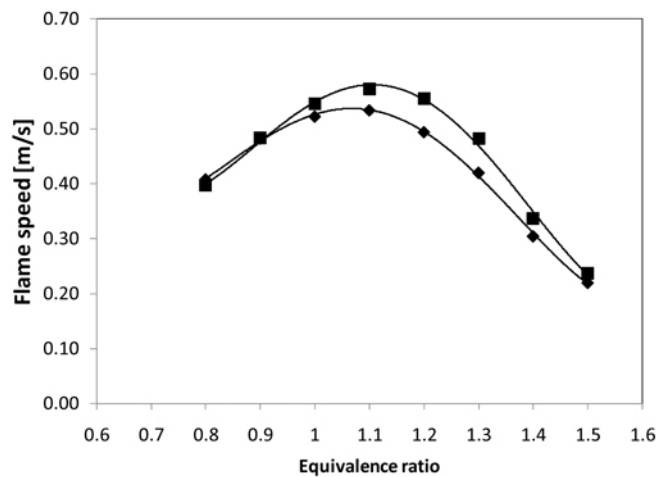


**Figure 3.** Comparison of complete ( $\text{—}\blacksquare\text{—}$ ) (LLNL) [12] and Andrae-Head mechanism ( $\text{—}\blacklozenge\text{—}$ ) for n-heptane at 325 K and 100 kPa.

Figures 4 and 5 show the comparison of experimental [27] and computational LFS of gasoline (CR-87) at 500 K and 353 K at 1 atm respectively. Again it is observed that the model is