Simulation of Laminar Burning Velocities for Alternative Fuels in SI Engines

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ABSTRACT

In the simulation of the spark ignition engine cycles, modelling of the turbulent flame propagation presents particular problems. Generally, turbulent flame propagation models are based on laminar burning velocity, turbulent intensity and one or more scale parameters of turbulence. A empirical model is presented for laminar burning velocity as a function of mixture strength, unburned mixture temperature, pressure, and residual gas fraction. Fuels considered include methane, ethanol, methanol, alcohol/water blends, isooctane/alcohol blends, propane and isooctane. Published data of other workers and the predictions of theoretical thermo-kinetic models have also been considered. It was noticed that in a constant unburned mixture temperature and equivalence ratio, arrangement for burning velocity of isooctane-methanol blends is methanol, isooctane, 90%isooctane/10%methanol and 80%isooctane/20%methanol. In isooctane-ethanol blends, results of simulation indicates which maximum burning velocity of ethanol is higher than 80%isooctane/20%ethanol, 90%isooctane/10%ethanol and isooctane. In constant circumstances maximum laminar burning velocity for equivalence ratio of 0.7-1.1 belong to blend of 80% isooctane(gasoline) and 20%ethanol while in equivalence ratio of 1.1-1.4 it belongs to ethanol.

Key Words: laminar burning velocity- empirical model- alternative fuels

1-INTRODUCTION

The knowledge of the fundamental properties of combustion is important because of the need to conserve fuel and protect the environment. Research into alternative fueled vehicles and power plants has increased interest in the fundamental combustion properties of a riety of gasoline alternatives. Of particular interests are the use of methane, the main component of compressed natural gas (CNG) and blending of gasoline-ethanol. As work continues on the development of CNG and bioethanol vehicles, simple, workable correlations are needed for the modelling of combustion over a wide range of temperaturesand pressures. One of the fundamental properties of fuel/air mixtures is its laminar burning velocity. It is used frequently for modeling turbulent flame propagation and pollutant formation in internal combustion engines. Values of burning velocity are needed over a large range of temperatures in modelling the combustion process of an internal combustion engine. Various forms of empirical and semiempirical functional relationships have been proposed for laminar burning velocity. The simplest form of the wholly empirical correlations which was adopted by several investigators [1-7] is:

$$S_U(\phi,T,P)=S_{U0}(\phi)[T_U/T_0]^{\alpha}[P/P_0]^{\beta} \tag{1}$$

Where S_{U0} is the velocity measured at $T_U=T_0$ and $P=P_0$ for a given mixture strength Ø, and α, β are constants or mixture strength dependent terms. Another empirical relation is the one proposed by Kuehl [8] for the propane-air mixtures:

$$S_U=\frac{7780(P/P_0)^{\beta}}{[\frac{10000}{T_f}+\frac{900}{T_U}]^{4.938}}(m/s) \tag{2}$$

Where T_f is the adiabatic flame temperature computed at P, T_U and given equivalence ratio Ø. The following empirical relation has been used to correlate the experimental data on stoichiometric isooctane, n-heptane and benzene-air mixtures [9]:

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$$S_U = (A.LnT_U - B).P^n \tag{3}$$

Where:

$$n = a + b(T_U / 1000) \tag{4}$$

And A, B, a and b are fuel dependent constants. For methane-air mixture equation (5) is proposed as following empirical expression:

$$S_U = [S_{U0} - 15.\phi.LogP].[T_U / 300]^m \tag{5}$$

Where:

$$S_{U0} = -418 + 1287/\phi - 1196/\phi^2 + 360/\phi^3 \tag{6}$$

And

$$\begin{aligned} m &= 1.68/\sqrt{\phi}\, for \phi \leq 1.0 \\ m &= 1.68.\sqrt{\phi}\, for \phi \geq 1.0 \end{aligned} \tag{7}$$

An expression similar to equation (1) was used to correlate the measured maximum flame velocities of isooctane,benzene and n-heptane-air mixtures for a wide range of initial mixture temperatures T_U , namely:

$$S_U = C_1 + C_2.T_u^{\alpha} \tag{8}$$

Where C_1 , C_2 and α are constants for the given fuel.

2- Modeling and Results

2-1- Laminar velocity at room temperature for methane

The majority of the experimental studies dealing with the determination of the laminar burning velocity have been devoted to methane-air mixtures and as aresult, there exists a considerable amount of data on burning characteristics of methane-air mixtures. Some of the data are shown in Figure 1. Burning velocity estimates of the thermokinetic combustion models yield values between 0.4 and 0.46 m/s for the maximum velocity of methane-air mixtures which are in good agreement with data of this study, results of this study showed that maximum velocity of methane-air mixtures is 0.418 m/s which occures in equivalence ratio of 1.1 at pressure of 1 atmospheric condition.

In this study, a new equation has been presented for calculation of laminar burning velocity of alternative fuels in spurg ignition engines. Equations of other researches have been modifieded for presenting of this equation. The following empirical expression has been chosen to represent the room temperature burning velocity of alternative fuels:

$$S_{U0}(\phi) = A.B.\phi^{\lambda}.\exp[-\psi.(\phi - 1.075)^2] \tag{9}$$

Where B, λ and ψ are constants for a given fuel, and A=1 for single constituent fuels. The constants for alternative fuels are listed in Table 1.

Burning velocity data in several amounts of equivalence ratio (Ø), unburned gas temperature (T_U) and pressure (P) variables in the following form has been used:

$$S_{U0}(\phi, T, P) = A.B.\phi^{\lambda}.\exp[-\psi.(\phi - 1.075)^2.[T_U / T_0]^{\alpha}.[P / P_0]^{\beta}(1 - \varphi.\mu) \tag{10}$$

The values of A, B, λ, ψ, α and β for different fuels have been evaluated and are tabulated in Tables 1, 2 and 3. The value of the constant φ may be taken 2.3-2.5 [16]. μ is the mole fraction of the inert diluent, for the range 0≤μ≤0.2, value of φ was determined as 2.1 by [3] and as 2.5 for 0≤μ≤0.3 by [16].

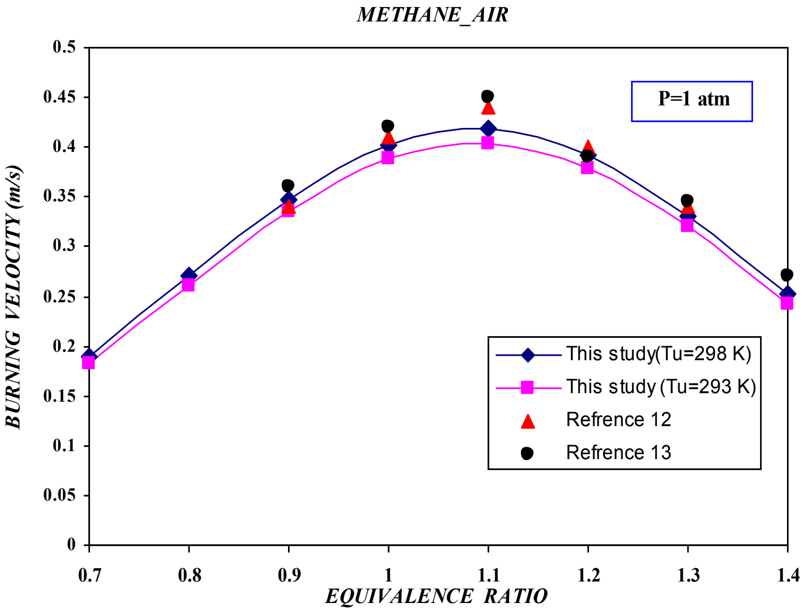

Figure 1- Laminar burning velocity of methane-air mixtures

Table 1- Values A, B, λ and ψ for equation (9): (T_{U0}=300 K, P_0= 100 kPa) [17].

FUEL	A	B	λ	ψ
METHANE	1	0.422	0.15	5.18
PROPANE	1	0.446	0.12	4.95
METHANOL	1	0.492	0.25	5.11
ETHANOL	1	0.465	0.25	6.34
ISOOCTANE	1	0.4658	-0.326	4.48
ISOOCTANE-MTHANOL	(1-0.53V)	0.4658	-0.326	4.48
ISOOCTANE-ETHANOL	$(1+0.07V^{0.35})$	0.4658	-0.326	4.48
ETHANOL-WATER	(1-3.25C_W)	0.465	0.25	6.34
V= volume (liquid) percent of alcohol in isooctane (Gasoline), $0 \le V \le 0.2$.				
C_W= mole fraction of water in stoichiometric fuel-air-water mixture.				

Table 2- Values of β for equation (10)(T_{U0}=300 K, P_0= 100 kPa) [17].

FUEL	Pressure exponent, β	
	ø≤1	ø ≥1
METHANE	-0.5	
PROPANE	-0.2	
METHANOL	$-0.2/\sqrt{\phi}$	-0.2ϕ
ETHANOL	$-0.17/\sqrt{\phi}$	$-0.17\sqrt{\phi}$
ISOOCTANE	-0.22	
ISOOCTANE-ALCOHOL	Similar to isooctane	
ETHANOL-WATER	0.28C_W-0.17	
$0.0 \le C_W \le 0.144$		

Table 3- Values of α for equation (10)(T_{U0}=300 K, P_0= 100 kPa) [1].

FUEL	Pressure exponent, α
METHANE	2
PROPANE	1.77
METHANOL	1.75
ETHANOL	1.75
ISOOCTANE	1.56
ISOOCTANE-METHANOL	1.55
ISOOCTANE- ETHANOL	$1.56+0.23V^{0.46}$ ($0.0 \le V \le 0.2$)
ETHANOL-WATER	1.75

2-2- Laminar velocity at room temperature for propane

Propane is an important combustion fuel and unlike hydrocarbon fuels with simple structures such as methane and ethane, the thermodynamical and combustion properties of propane are similar in many ways to those of more complex practical fuels. For this reason, it is often used in laboratory studies of oxidanation processes in internal combustion engines, detonations and other environmental. Equation (10) has been used to correlate room temperature and atmospheric pressure data; and results of this simulation for propane has been indicated in Figure 2. For propane, maximum of the laminar burning velocity is 0.4198 m/s which accures in 1.1 equivalence ratio. Results of this study are in agreement with the results of refrences [14] and [15].

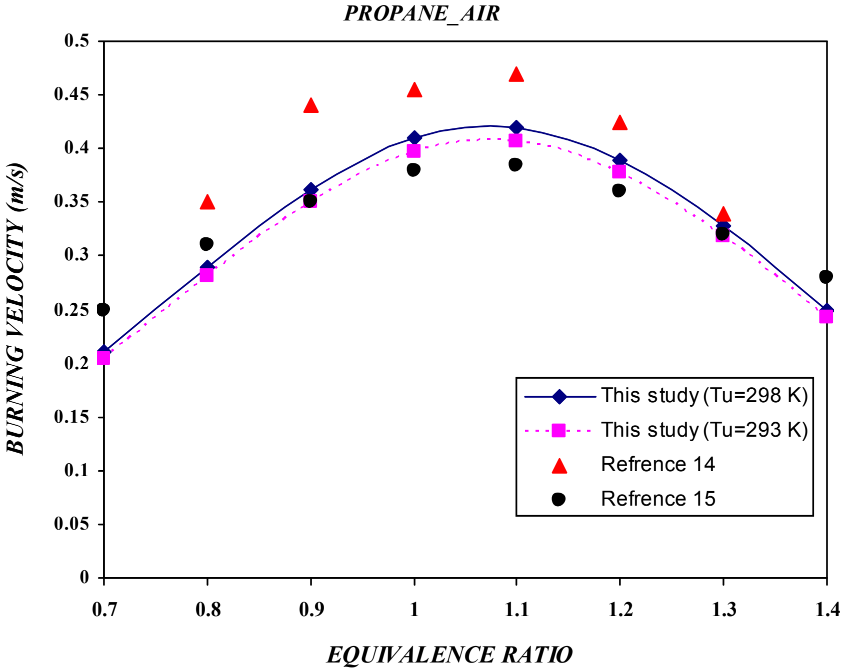

Figure 2- Laminar burning velocity of propane-air mixtures

2-3- Laminar velocity at room temperature for isooctane

Although isooctane has been widely used in spark ignition engine research to simulate gasoline, it has not been studied as much as methane or propane for its fundamental combustion characteristics. Simulation 's data available in the combustion literature are shown in Figure 3 along with simulation of this study. For isooctane, maximum of the laminar burning velocity is 0.454 m/s which accures in 1 equivalence ratio.

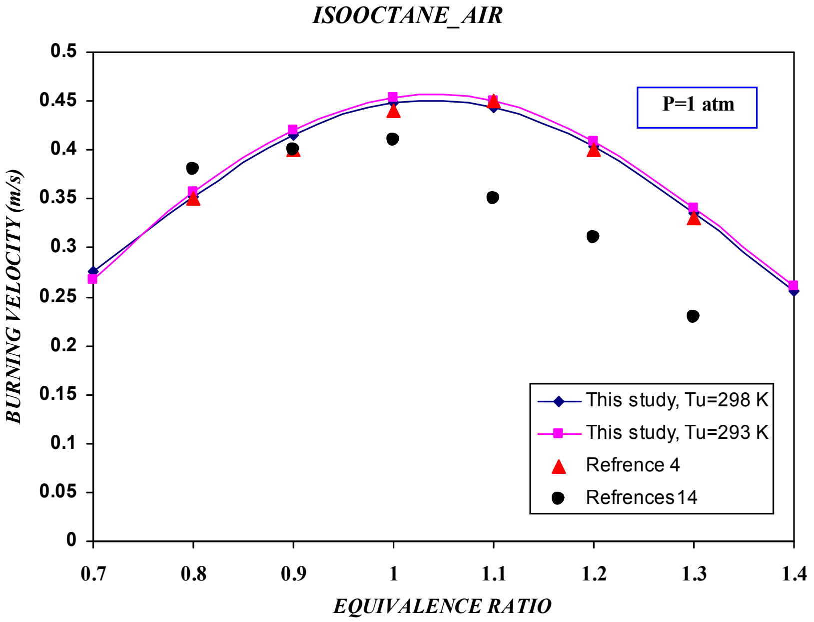

Figure 3- Laminar burning velocity of isooctane -air mixtures

2-4- Laminar velocity at room temperature for methanol

Althogh methanol applications as a spark ignition engine fuel have recently received much attention, fundamental experimental data on combustion characteristics of methanol are very limited; in particular, only a few studies have been reported for high pressure and temperature conditions. Available room temperature burning velocity data for methanol with those of the present authors [4] and [14] are replotted in Figure 4. Constants of equation (10) for methanol-air mixtures have been determined mostly using the data which are given in Table 1. Formethanol, maximum of the laminar burning velocity is 0.494 m/s which accures in 1.1 equivalence ratio.

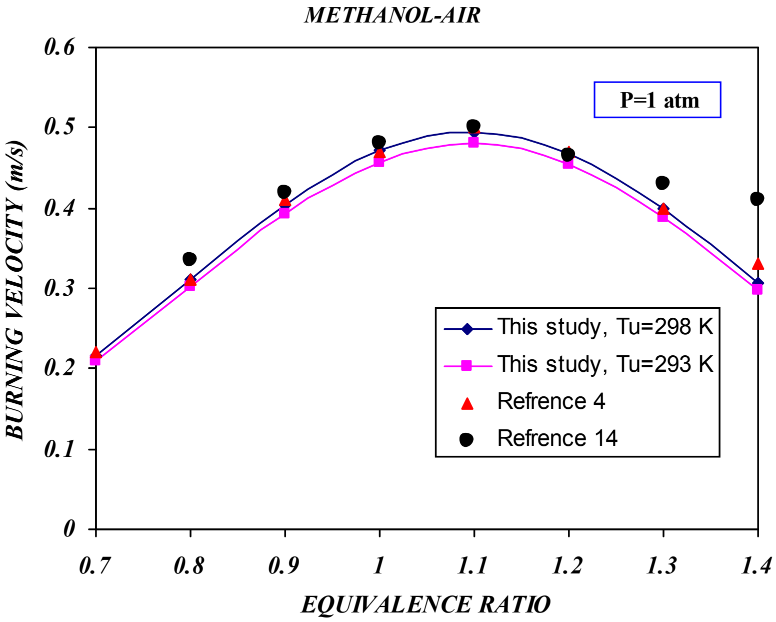

Figure 4- Laminar burning velocity of methanol-air mixtures

2-5- Laminar velocity at room temperature for ethanol

Published laminar burning velocity data of ethanol-air mixtures are limited to two studies. An early work reported the maximum burning velocity of ethanol-air mixtures at 100°C as 0.79 m/s at an equivalence ratio ø=1.1 [18]. Recently a more detailed study has been reported by the present author [4]. These data are plotted in Figure 5 as a function of equivalence ratio. Constants of equation (10) for the estimation of the burning velocities of ethanol-air mixtures under atmospheric conditions are listed in Table 1.

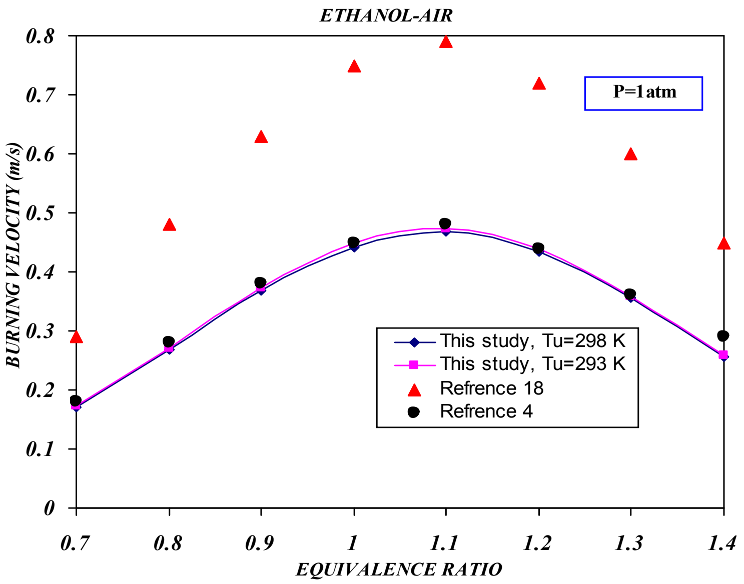

Figure 5- Laminar burning velocity of ethanol-air mixtures

2-6- Laminar velocity at room temperature for alcohol-isooctane blends

Although the majority of alcohol fuel applications in internal combustion engines, at present are in the form of hydrocarbon-alcohol blends. A decrease in ignition delay and in flame travel time was observed in S.I. engines fueled with alcohols, however it was found that, under certain conditions, flame travel is longer with gasoline-alcohol blends as compared to that of gasoline. This observation raises the question whether the burning velocities of multiple fuel mixtures can be predicted by simple mixing rules. There exists a number of burning velocity prediction techniques for multicomponent gaseous fuel mixtures. However it has been shown recently that no existing technique for multicomponent fuel gas is reliable. It should be noted that available thechniques were based on thermal consideration and that they do not account for any chemical kinetic interactions. Although the effects of alcohol addition to gasoline on engine performance and exhaust emission have been studied by several investigators, the results obtained seem to be contradictory in some cases. A major drawback is the lack of fundamental combustion data for alcohol-hydrocarbon mixtures which are essential for theoretical predictions to support the experimental findings [17]. Figure 6 showes the burning velocities of the several ethanol-gasoline blends as compared to those of gasoline and ethanol. Burning velocity of methanol-gasoline blends are shown in Figure 7.

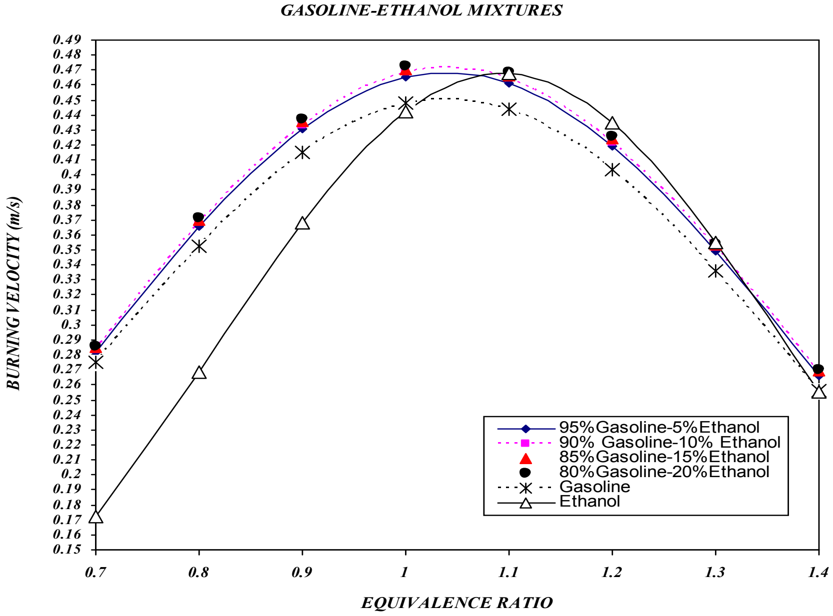

Figure 6- Laminar burning velocity of ethanol-gasoline mixtures

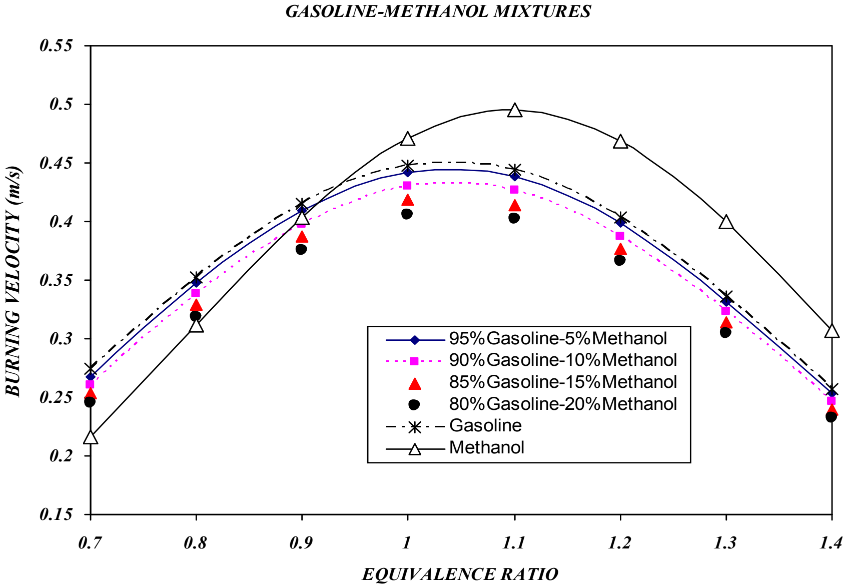

Figure 7- Laminar burning velocity of methanol-gasoline mixtures

In order to show the effect of alcohol addition to isooctane on burning velocity a comparison is made in Figure 8. Results indicates that after of equivalence ratio 1, burning velocity of ethanol is higher than other ethanol-gasoline and methanol-gasoline blends but before of 1, maximum burning velocity belong to 20%ethanol and 80% gasoline blend.

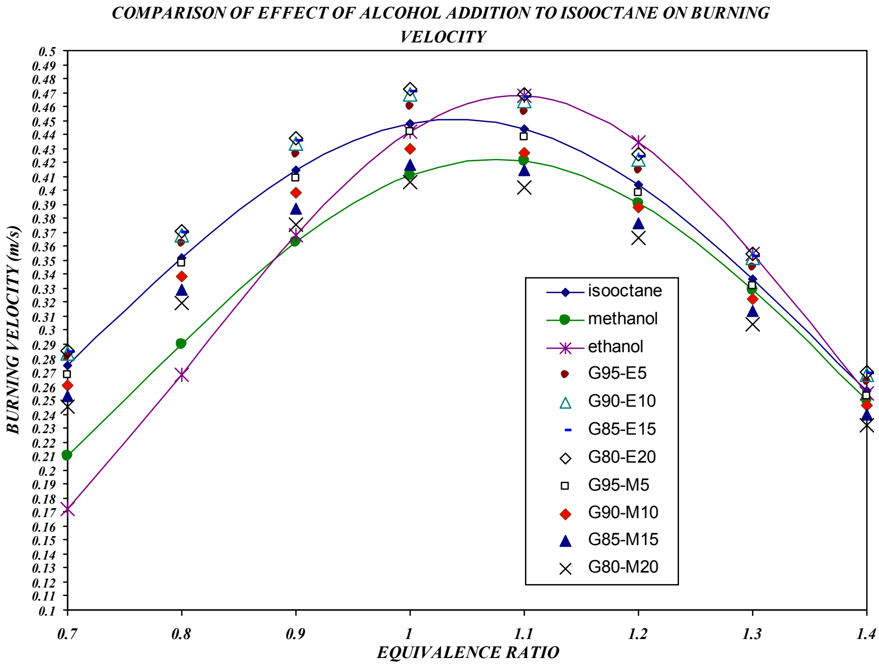

Figure 8- Comparison of Laminar burning velocity for methanol-gasoline and ethanol-gasoline mixtures

2-7- Laminar velocity at room temperature for alcohol-water mixtures

The use of water as an ancillary combustion control technique has received much interest since the beginning of this century [17]. The observed effects in internal combustion engines were internal cooling and elimination of detonation and preignition. The major motivation in the last two decades has been the reduction of combustion-generated nitric oxide emissions by water addition. Alcohol-water mixtures as fuels were considered in order to decrease nitric oxide emissions in spark ignition engines and to boost the octane quality of the alcohol fuel for application in high compression ratio engines to achieve higher conversion efficiencies. It has been long known that trace amounts of water vapor accelerates the carbon monoxide combustion [17]. However, laminar methanol-air and hydrogen-air flames are inhibited by water vapor addition [13]. Figure 9 shows the effect of water concentration on burning velocity at different equivalence ratio.

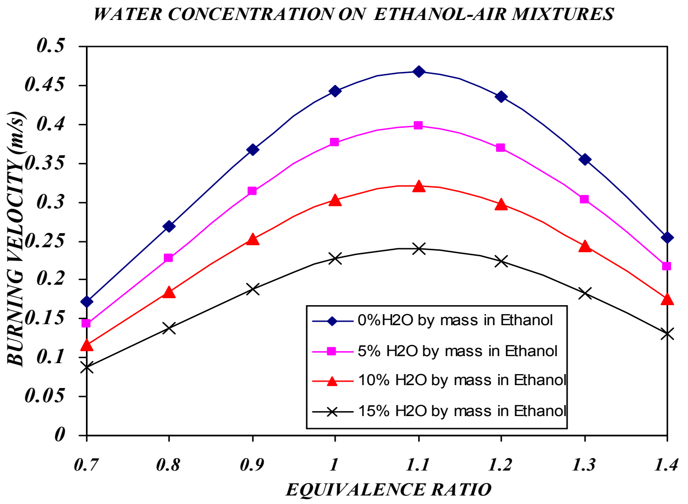

Figure 9- Effect of water concentration on burning velocity of ethanol-air mixtures

3-Conclusions

Burning velocity data of different alternative spark ignition engine fuels, obtained by several workers and in this present study. Fuels considered include ethanol, methanol, alcohol-water blends, isooctane-alcohol blends, propane, methane and isooctane. An empirical expression in the following form has been used to correlate the burning velocity data:

$$S_{U0}(\phi,T,P)=S_{U0}(\phi).[T_U/T_0]^{\alpha}.[P/P_0]^{\beta}(1-\varphi.\mu)$$

Where:

$$S_{U0}(\phi)=A.B.\phi^{\lambda}.\exp[-\psi.(\phi-1.075)^2]$$

The values of A, B, λ, ψ, α and β for different fuels have been evaluated and are tabulated in Tables1, 2 and 3. The burning velocity data of various workers are compared with results of this study and it indicated that there is a good adaption between data. Although, the burning velocity data of various workers are compared with results of this study, the details related to the measurement and data evaluation techniques are not covered in this paper. Figure 10 indicates laminar burning velocity of alternative fuels in spark ignition engine, maximum burning velocity belong to blending of 80% gasoline and 20% ethanol while minimum of this amount belong to 80% gasoline, 20% methanol blend of fuel.

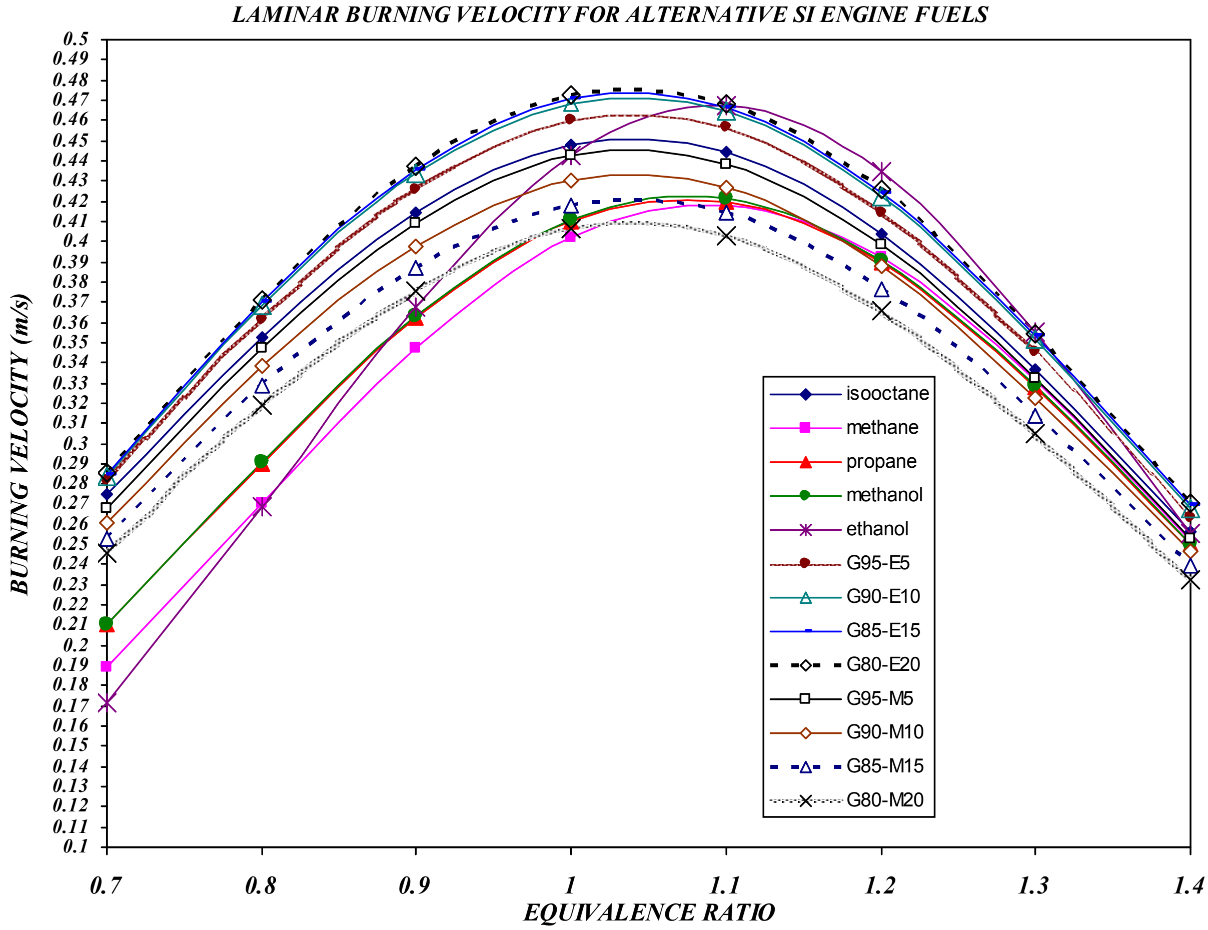

Figure 10- Laminar burning velocity for 13 alternative SI engine fuels

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