PSFC/JA-05-21

In-Cylinder Laminar Flame Propagation Speed: Effect of Hydrogen And Hydrogen Rich Gas Addition

L. Bromberg

August 26, 2005

MIT Plasma Science and Fusion Center

Abstract

In this paper, the implication of various grades of hydrogen rich gas on the in-cylinder flame speed, and on the knock propensity, are discussed. The laminar flame propagation speed of methane with various grades of hydrogen-rich gas addition has been calculated. The effect of adding hydrogen, hydrogen rich gas from an ideal reformer (synthesis gas), as well as that from a non-catalytic plasmatron fuel reformer has been determined. The model has been used for stoichiometric as well as lean combustion. The effect of including the enthalpy of the reformate on the both the flame speed and on the propensity to knock has also been considered. A simple formula for the calculation of the flame speed for the case of mixtures of reformate and conventional fuels is proposed and has been tested against experiments at atmospheric pressure with hydrogen enriched flames.

1. Introduction

Application of hydrogen rich gas addition for ignition stability has been proposed for high efficiency SI vehicles [1-16]. The effect is attributed to the increased speed of flame propagation that results with the introduction of hydrogen or hydrogen rich gas. The main effect is the ability to operate lean and unthrottled in a SI engine. In addition, hydrogen has been shown to allow operation at increased compression ratio because of the ability of hydrogen rich gas to prevent knock (high octane) [17].

The main effect of hydrogen addition in SI engines has been the increase of the 0-10% burn of the fuel, with no noticeable effect on the 10-90% [14,15]. During this phase the laminar flame speed dominates the combustion process. A case can be made that the 0-10% burn rate, and maybe even the misfire characteristics of the engine/fuel combination, are associated with the laminar flame speed.

Since during the 0-10% burn of the fuel the pressure in the cylinder is not varying much, the effect in the flame speed of hydrogen addition can be readily calculated. The turbulent flame propagation and knock phenomena occurs later in the fuel burn.

The calculation of the laminar flame propagation speed may provide guidance to the tradeoffs between reformate temperature, hydrogen purity and the effect of other compounds (such as water and carbon dioxide) that are generated when using a homogeneous plasmatron fuel reformer.

In this paper a chemical kinetics code is used to determine the laminar flame propagation speed. Section 2 describes the chemical kinetic model. Section 3 shows the chemical kinetic calculations for air/methane mixtures, while section 4 reviews recent experiments and calculations of laminar flame speeds of isooctane/hydrogen and isooctane/reformate fuels [18]. The experimental results from Huang [18] are used to propose a formula that can be used to easily calculate the flame speed of a mixture of fuels. The simple formula is tested in the rest of the paper for other fuel mixtures that include fuel mixtures of methane, hydrogen, synthesis gas and reformate from plasmatron gasoline converters. Section 4 also describes the difficulty in defining the equivalence ratio in fuels that contain reformate, and in particular reformate from partial oxidation reformers. Two definitions of the equivalence ratio, used throughout the paper, are described.

Section 5 presents results from flame speed calculations of stoichiometric air/methane/hydrogen mixtures, while section 6 shows results for air/methane/synthesis gas mixtures (ideal reformate). In section 7 reformate typical from plasmatron gasoline reformers is used.

The calculations from section 4 to Section 7 are for stoichiometric air/fuel mixtures. Section 8 presents results of flame speed calculations for lean operation with the addition of plasmatron gasoline reformate. Both the effects on the laminar flame speed of the composition of the air fuel mixtures, as well as the thermal content of the reformate, are investigated. Section 9 briefly describes the knock consequences of injecting cold or hot

reformate, both at stoichiometric and lean conditions, at conditions of low speed, high torque. This section describes the results for gasoline, not for methane. Finally, Section 10 summarizes the work and gives the conclusions.

2. Description of the model

The flame speed module in the CHEMKIN 4.0 package was used [19]. An attempt was made to use a PRF mechanism, but the mechanism was too large for the CHEMKIN code (although a recent release of the CHEMKIN 4.0.2 package solves this problem). In this paper, it was assumed that the primary fuel was methane. The chemistry, thermodynamic and transport mechanisms used in the simulations is the GRI 3.0 [20]. In addition, the methane mechanism is better established than isooctane.

Methane has a relatively high flame speed, compared with gasoline. However, it is expected that the trends of the effect of temperature, hydrogen or hydrogen rich gas, and composition of the reformate will carry over to the case of isooctane, which will be investigated later.

Unless otherwise noted, the laminar flames propagation speed is calculated at a pressure of 17 bar and a temperature of 640K (*i.e.*, spark timing before TDC). This corresponds to naturally aspirated engine with a compression ratio of 10, with an air inlet of 375 K.
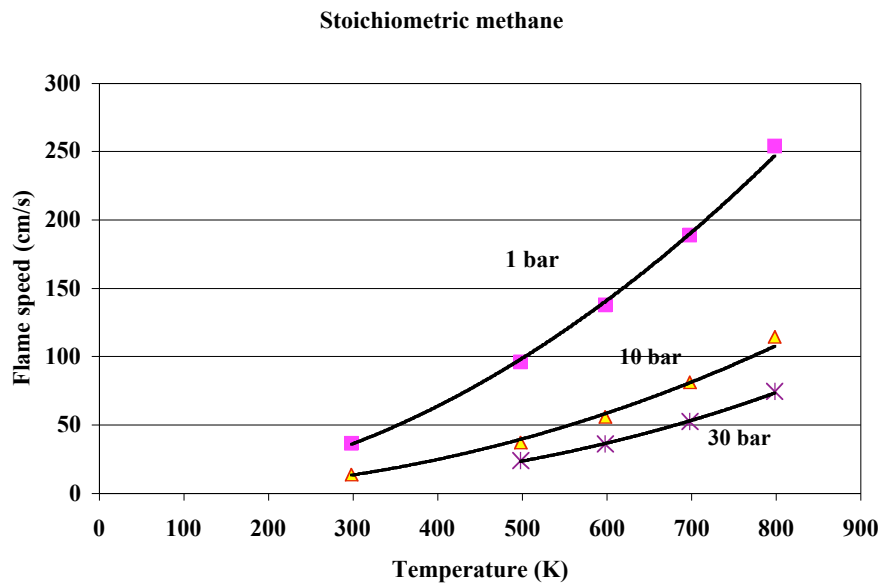

Figure 1. Flame speed for stoichiometric air/methane mixture as a function of initial air/methane temperature, for several operating pressures.

3 Laminar flame propagation speed of stoichiomertic air/methane mixtures

The calculated laminar flame propagation speeds of stoichiometric air/methane mixtures are shown in Figures 1 and 2. Figure 1 shows at constant pressure as a function of

temperature, while Figure 2 shows constant temperature as a function of pressure. Higher pressure decreases the flame speed, higher temperature increase it. The flame speed is on the order of 10's of cm/s.

The pressure dependence (at constant temperature) is on the form $v \sim 1/p^{1/\alpha}$, where α is ~ 2.5 at 498K to 2.8 at 798K.   Similarly, the temperature dependence (at constant pressure) is $V \sim T^{\beta}$, where $\beta \sim 2$ for 1 bar and 2.4 for 30 bar.
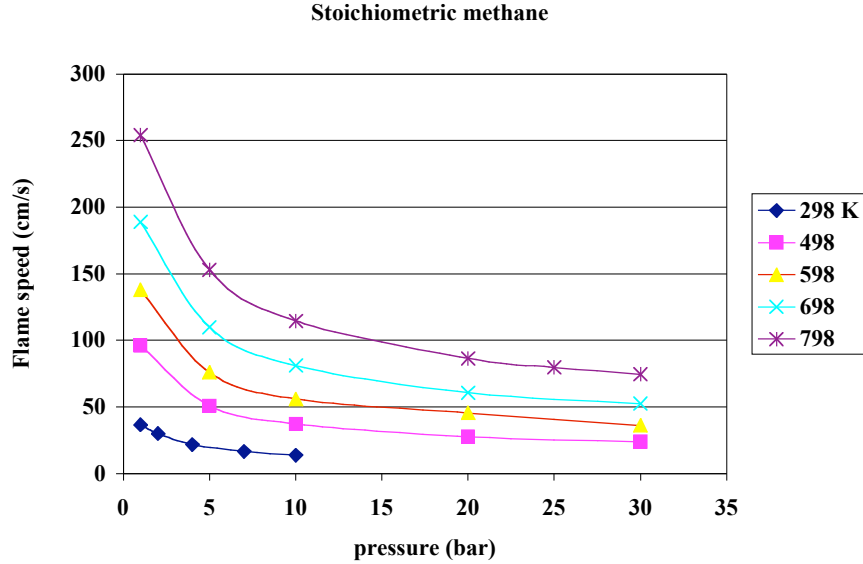
Stoichiometric methane

Figure 2. Same as Figure 1, but shown for constant temperature as a function of the pressure.

4 Flame speed of isooctane/reformate gas mixtures, and approximate formula

The flame speed of isooctane reformate mixtures has been measured by Huang *et al.* [17]. The purpose of this section is to determine a method of predicting the flame velocity of the mixtures used in those experiments, in order to provide an algorithm that can be tested in the calculations presented in later sections of this paper.

Huang *et al.* [18] measured the flame speed of isootance/reformate gas mixtures at atmospheric pressure and room temperature. The experiments were performed by varying the ratio of the isooctane to total fuel fraction (isooctane plus reformate) while holding constant the equivalence ratio ϕ_m, defined as the ratio between the amount of air required to oxidize the isooctane/reformer gas mixture and the amount of air introduced in the system.
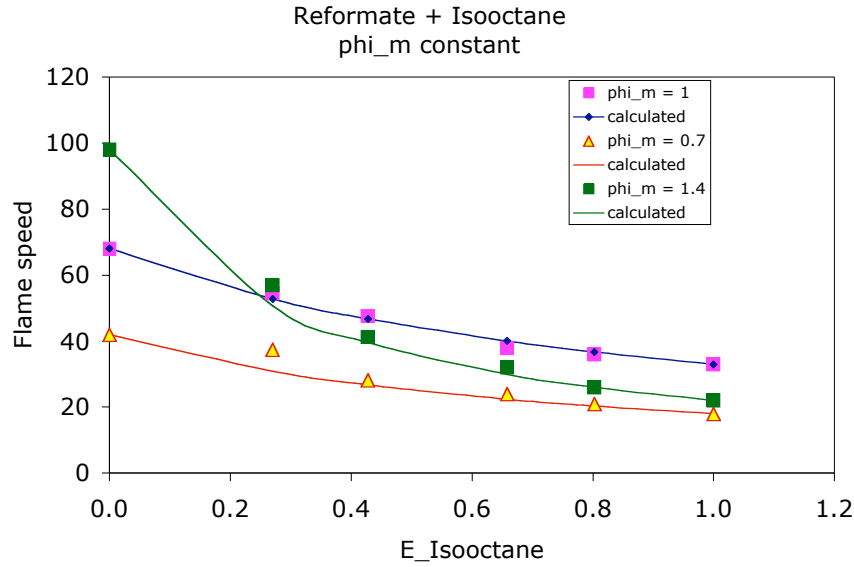
Figure 3. Experimental flame speed of isooctane-reformate mixtures as a function of the fraction of the isooctane energy fraction, for constant values of ϕ_m. (points using experimental data of Huang [18]); also plotted is $v_{mixture}$ (solid curves) using eq (1).

We have processed Huang's experimental results [18] to determine the fraction of the energy provided by the hydrocarbon fuel and to determine the value of the equivalence ratio that a lambda sensor would measure in the combustion products, which includes the air used to reform the fuel, $\phi_{exhaust}$. It should be noted that the definitions of $\phi_{exhaust}$ and ϕ_m are the same for equivalence ratios of 1, but differ for other values. Physically, the air used to generate the reformate is included in the definition of $\phi_{exhaust}$ but not in the definition of ϕ_m. $\phi_{exhaust}$ includes the nitrogen in the air used in the reformer (which becomes a diluent in the combustion zone. The energy lost in the reformation process in not included in either definition.

We propose that the flame propagation speed of a mixture follows an inverse rule weighed by energy content, i.e., the flame velocity of the fuel mixture follows the following relationship:

$$1/v_{mixture} = F_{RG}/v_{RG} + (1-F_{RG})/v_{isooctane} \qquad (1)$$

In eq (1) F_{RG} is the energy fraction of the fuel in the reformer, and v_{RG} and $v_{isooctane}$ are the flame speeds for unmixed reformer gas and isooctane, respectively, at the given value of either ϕ_m or $\phi_{exhaust}$. This formula will be referred to in the text as the inverse-speed energy weighted laminar flame propagation speed equation.

Figure 3 and 4 show the experimental results of Huang [18] (solid points) and of the simple relationship described above in eq (1) (solid lines). The experimental results in Figure 2 are plotted against the estimated values of the energy fraction in the isooctane, E_Isooctane, for different value of ϕ_m (calculated from data in the paper by Huang [18]).

The values of the flame velocity for reformer gas and isooctane are taken from the extremes of the curves, so the curve automatically fits that part of the curves well.
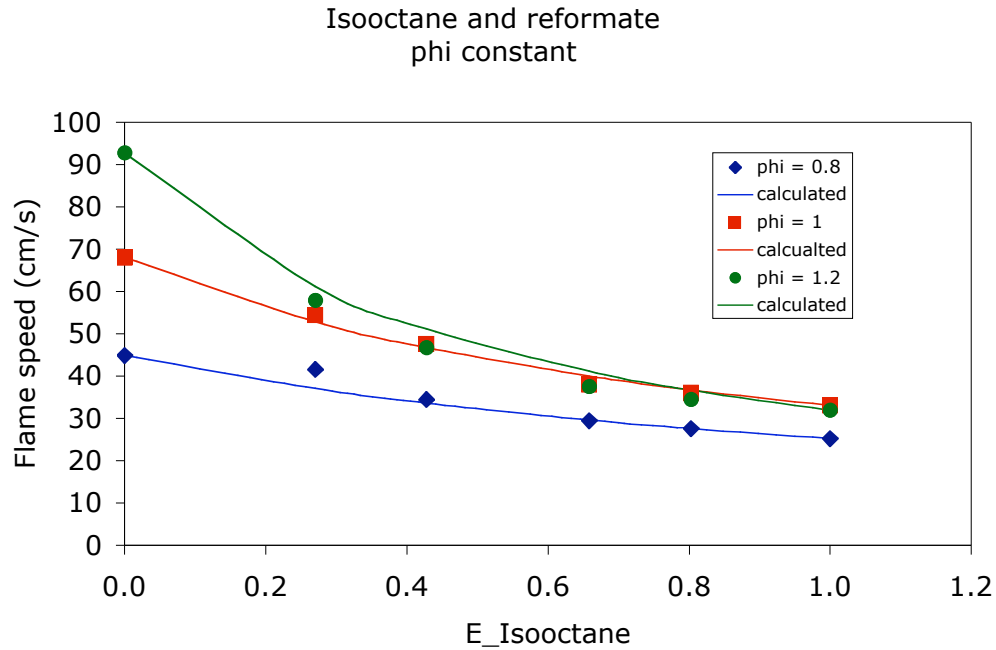

Figure 4.   Interpolated experimental values of flame speed (from results of Huang [18]) of isooctane-reformate gas mixtures, for constant values of $\phi_{exhaust}$ as a function of the isooctane energy fraction; also plotted is $v_{mixture}$ (solid curves) using eq (1).

Figure 4 shows the curve for extrapolated values of flame speed for constant value of $\phi_{exhaust}$. The experimentally determined values where fit to a quadratic curve, and values of flame speed at $\phi_{exhaust} = 0.8$ and 1.2 where determined by interpolation.

From the data and by comparing Figures 3 and 4 it is hard to determine which definition of equivalence ratio is more appropriate for calculating the flame speed. The data using ϕ_m constant (as done by Huang [18]) fits the experimental data better for rich combustion ($\phi_m > 1$). However, the extrapolation to fuel rich conditions involved larger errors than to fuel-lean conditions. The fuel lean region fit was better using $\phi_{exhaust}$ constant.

The laminar flame speed measurements by Huang [18] were performed at atmospheric conditions and at room temperature. Those results are not directly relevant to in-cylinder combustion, but they provide a frame for investigating the impact of hydrogen and reformate addition. An the next section, the effect on laminar flame speed of adding hydrogen to methane in a cylinder is calculated.

5 Laminar flame propagation speed with hydrogen addition

The first case studied is that of addition of pure hydrogen to the air/methane mixture to calculate the in-cylinder laminar flame propagation speed. A, conditions are 17 bar and

640 K. As the amount of hydrogen is increased, the amount of methane needs to be reduced to maintain stoichiometric conditions.

Stoichiometric (Hythane)
640 K, 17 bar

(a)

Stoichiometric H2 addition (HYTHANE)
640 K 17 bar
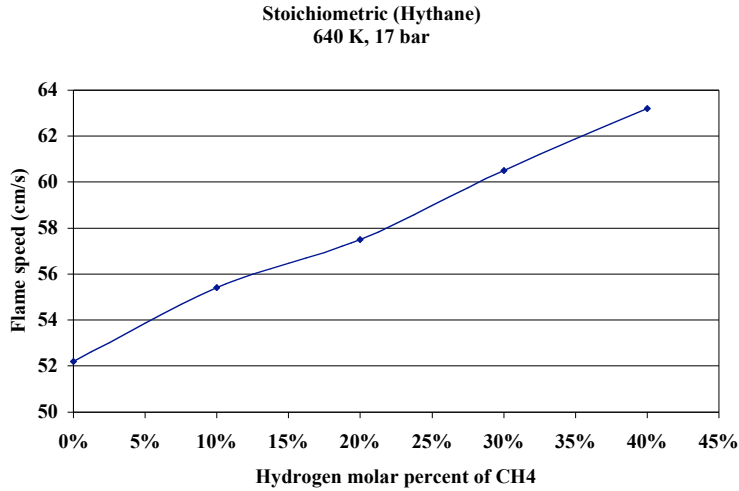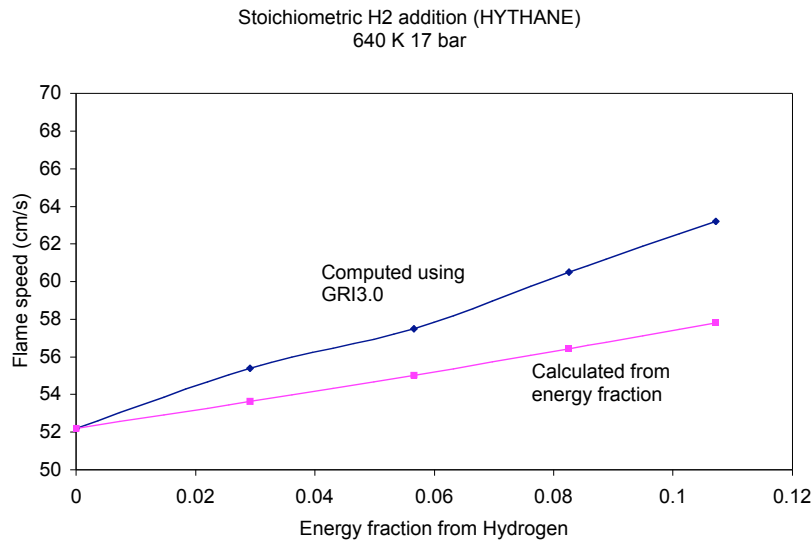
(b)

Figure 5. (a) Laminar flame speed (a) as a function of hydrogen to methane molar ratios; (b) as a function of the energy fraction of the fuel provided by the hydrogen. 17 bar, 640 K stoichiometric air/methane/hydrogen mixtures

The calculated flame speeds are shown in Figure 5. Although the flame speed increases, even for relatively aggressive hydrogen concentrations the flame speed does not increase more than about 20% (from 52 to 62 cm/s). Hythane, a mixture of hydrogen and methane that has been proposed as means of introducing of hydrogen, has a molar concentration of 30% hydrogen. Figure 5b shows the computed values of the flame speed of the mixture as a function of the energy fraction provided by hydrogen. Also shown are the values of the flame speed calculated using the inverse/energy fraction weighted equation found in the previous section. There is qualitative agreement between the two.

The flame speed of 100% hydrogen was calculated, and it was found to be 560 cm/s for the conditions of Figure 5. (At these conditions, the hydrogen/air mixture is explosive and the propagation is due to the formation of a shock).

It is not clear the effect of a 20% increase of the laminar flame speed on the combustion stability. It is guessed that the 0-10% burn time duration would be decreased accordingly.

**6 Flame speed with reformate addition: stoichiometric combustion**

In a fuel reformer such as the plasmatron fuel reformer [21-24], the fuel is converted to hydrogen and carbon monoxide (synthesis gas) under the process of partial oxidation. For ideal methane partial oxidation, the reaction is as follows:

$$CH_4 + 1/2\ O_2 + 3.76/2\ N_2 \rightarrow CO + 2\ H_2 + 3.76/2\ N_2$$
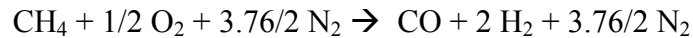
The concentration of the reformate from an ideal methane partial oxidation reformer is $CO/H_2/N_2$:1/2/1.88.

The laminar flame propagation speed with the addition of reformate to the air/methane mixture is shown in Figure 6. As in the previous section, the composition is adjusted so that the air/methane/reformate mixture is stoichiometric. It is assumed that the reformate is added at the same temperature as the methane/air (375 K). The effect of the introducing the reformate at higher temperature, made possible by the exothermic reactions in the reformer, will be discussed in a later section..

Figures 6 (a) and (b) shows the profiles across the flame for the case of 20% of the methane processed through an ideal reformer. These figures show the method of calculation of the laminar flame propagation speed. The flame is assumed stationary (at about 0.5 cm), and the flow rate of the unburnt air/fuel mixture calculated that results in a stationary flame (an eigenvalue problem). Figure 6(a) shows the spatial gas composition in front and behind the flame. Figure 6(b) shows the gas speed corresponding to the gas composition in Figure 6(a). Note the different spatial scale in Figures 6(a) and 6(b). At the left of the flame front, the gas speed (unreacted air/fuel mixture) is the flame speed. The velocity of the gas is much larger to the right of the flame, as a result of the increased gas temperature. The thickness of the flame front is very small, on the order of 0.003 cm (30 μm).
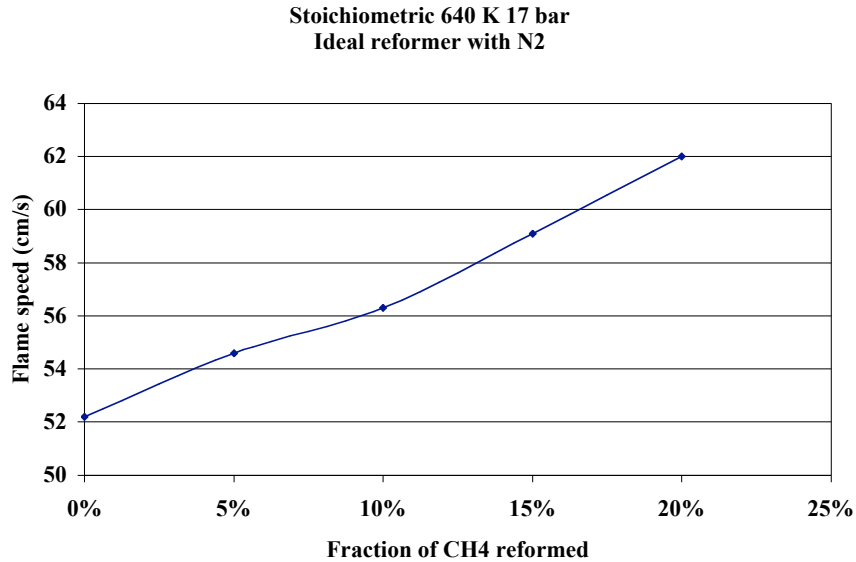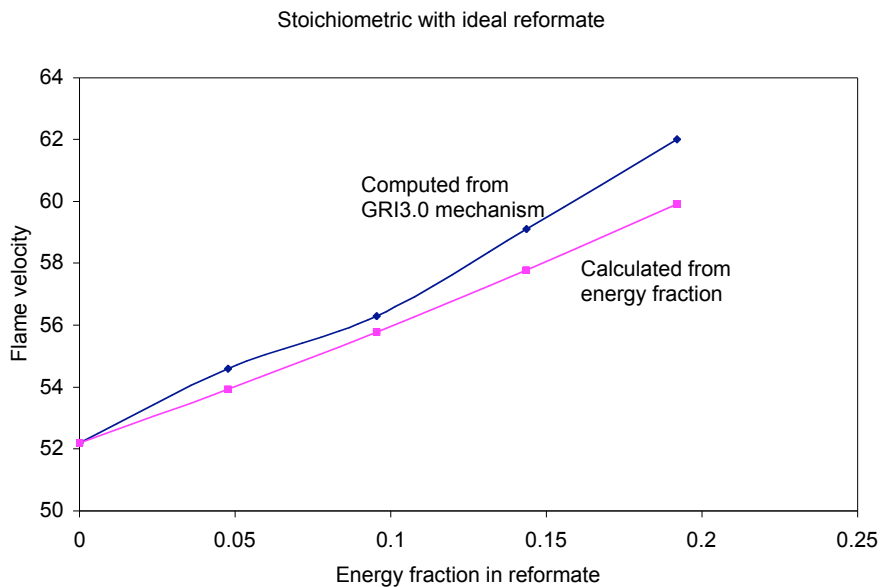
CHEMKIN Solution

(a)

CHEMKIN Solution
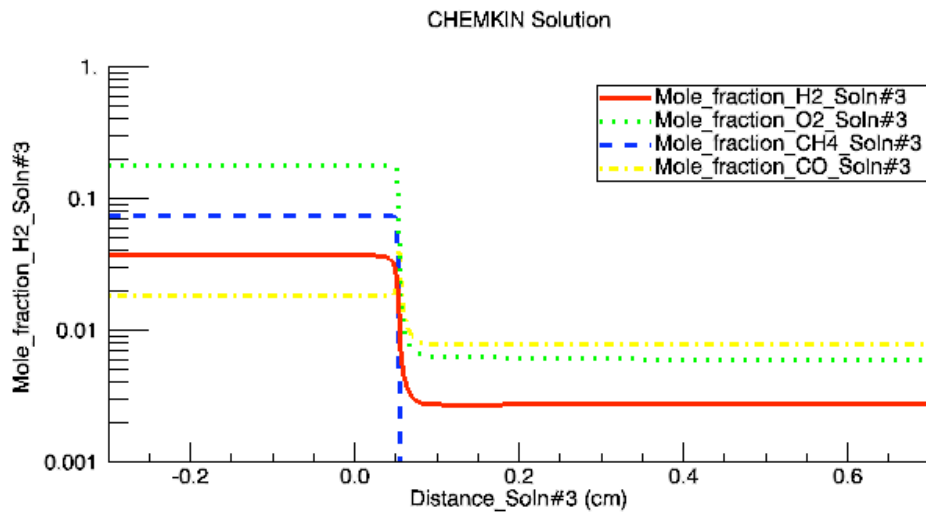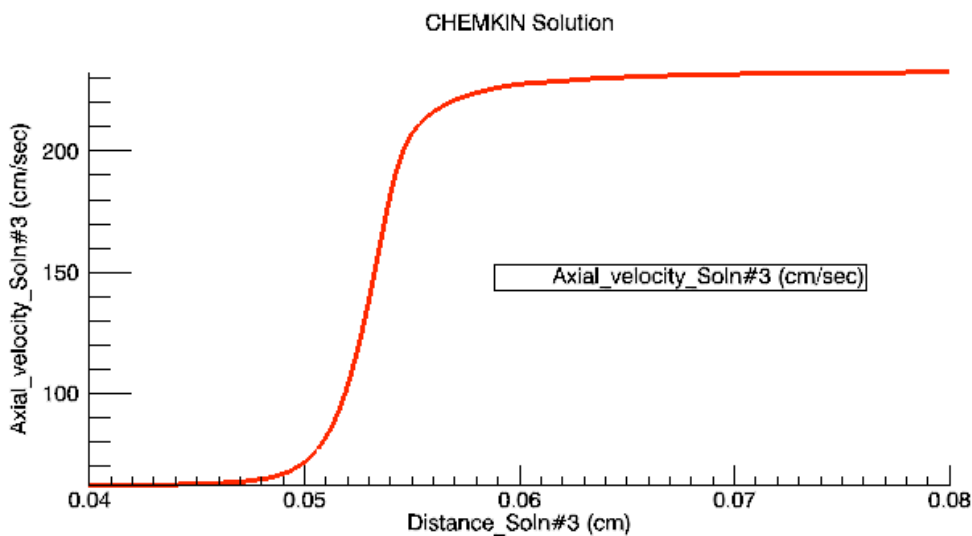
(b)

Figure 6. Characteristics of the air/methane/reformate laminar flame speed calculations: (a) composition of the gas (unburnt fuel to the left of the flame, burnt to the right) (b) gas velocity.

Figure 7(a) shows the laminar flame propagation speed as a function of the fraction of the fuel that is processed by the reformer. For pure hydrogen addition (discussed in the previous section) the hydrogen concentration in the gas is 2.6% for a 30% H_2 to CH_4 energy ratio in Figure 5a, with a corresponding laminar flame speed of 60 cm/s. This compares with a flame speed of 59 cm/s for a hydrogen concentration of 2.8% for the fraction of CH_4 reformed of 15% in Figure 7(a). The effect of hydrogen on the flame speed is smaller in the case of synthesis gas as opposed to just hydrogen, even in the cases of comparable concentrations of hydrogen. It should be stressed that the concentration of the other gases, including oxygen, are varying in this comparison. Figure

7(b) shows the data from Figure 7(a) as a function of the energy provided by the reformate, as well as the calculated values using the inverse/energy fraction weighted flame speed. The flame speed for 100% reformate is 160 cm/s.

Stoichiometric 640 K 17 bar
Ideal reformer with N2

(a)

Stoichiometric with ideal reformate

(b)

Figure 7. (a) Laminar flame propagation speed after addition of ideal reformate to air/methane mixture; 17 bar, 640 K, stoichiometric conditions (a) as a function of reformed CH_4 fraction (b) as a function of the energy fraction provided by the reformate

Figure 7(b) also shows the inverse-energy weighed $v_{mixture}$ calculated from eq (1). There is quantitative agreement between the kinetic calculations and the proposed equation for the flame speed of the mixture.

7 Flame speed with plasmatron reformate: stoichiometric combustion

The plasmatron fuel reformer, when operating without a catalyst, produces the composition shown in Table 1 [21]. The table is the results of experiments for gasoline. The data in Table 1 corresponds to a flow rate of fuel into the plasmatron of 0.95 g/s, with an O/C ratio of 1.13. Some of the fuel is fully combusted, with the presence of water and CO_2 in the reformate.

Table 1.
Composition of the reformate from the plasmatron fuel converter
(operating in gasoline) with metallic packing

H2	15.80%
CO	18.80%
CO2	3.30%
N2	55.70%
CH4	2.50%
C2H4	0.50%
C2H2	0.00%
O2	0.71%
H2O	2.77%

Because the plasmatron reformer is operated in gasoline but the laminar flame propagation speed calculations are performed for methane, the parameter used in this section to indicate the fuel/reformate fraction is the fraction of the oxygen that is combusted by the reformate, as opposed to the fraction of the fuel processed by the reformer. However, the results approximately correspond to the amount of the fuel that would be processed by the reformer.

Figure 8 shows the main compounds of the air/fuel mixture (balance is nitrogen) for the case of stoichiometric air/methane/reformate, for the experimentally determined reformate composition when using the plasmatron gasoline reformer. In this case the hydrogen and CO concentrations in the reformate and in the air/fuel mixture are comparable, since the ratio of hydrogen to carbon in the fuel (gasoline) is ~ 2:1, instead of 4:1 as in the case of methane. The concentration of oxygen decreases because of the diluting effect of the methane and gaseous reformate.

Figure 9 shows the corresponding flame speed for the stoichiometric combustion of air/methane/reformate mixtures, as a function of the energy fraction provided by the reformate. The flame speed actually decreases with the addition of the hydrogen rich gas. We think that the reason for the decrease is the large amount of CO_2 and water injected with the reformate, as well as the nitrogen diluent in the reformate gas. It follows that combustion stability would then actually decrease with the addition of the gasoline reformate with the composition in Table 1. It is not clear what the effect would be on

cylinder combustion stability, since the addition of reformate lowers the flame speeds from that of just methane. Also shown in Figure 9 is the inverse-energy weighted flame speed calculation. It should be noted that although the agreement is not great, the flame speed variation through this range is small.
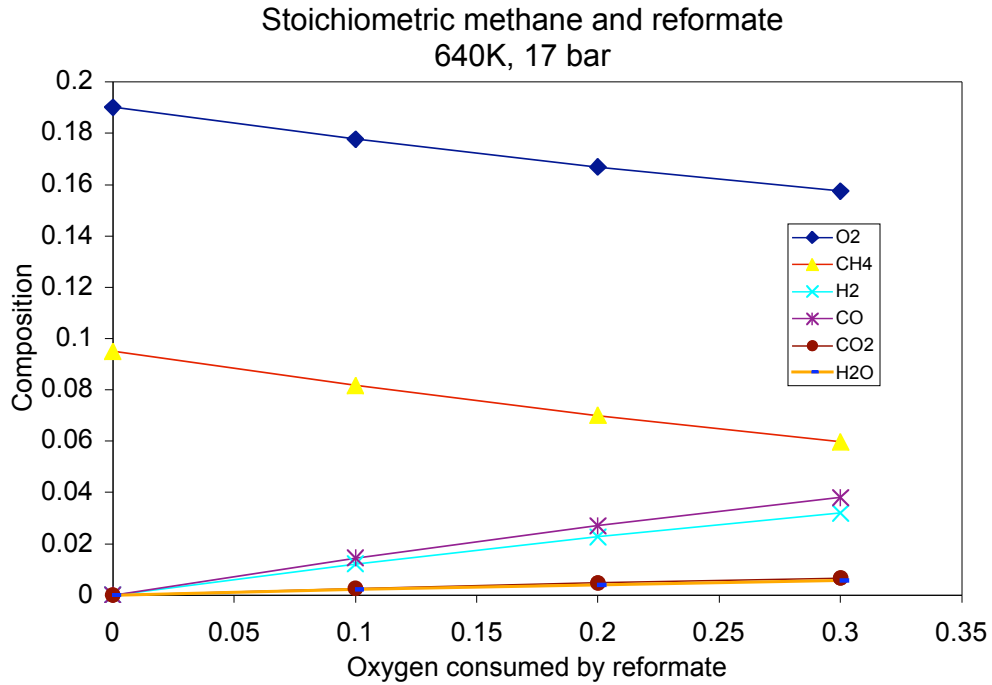
Figure 8. Composition of the stoichiometric air/methane/reformate mixture (balance nitrogen) as a function of the oxygen that is combusted by the plasmatron reformate.
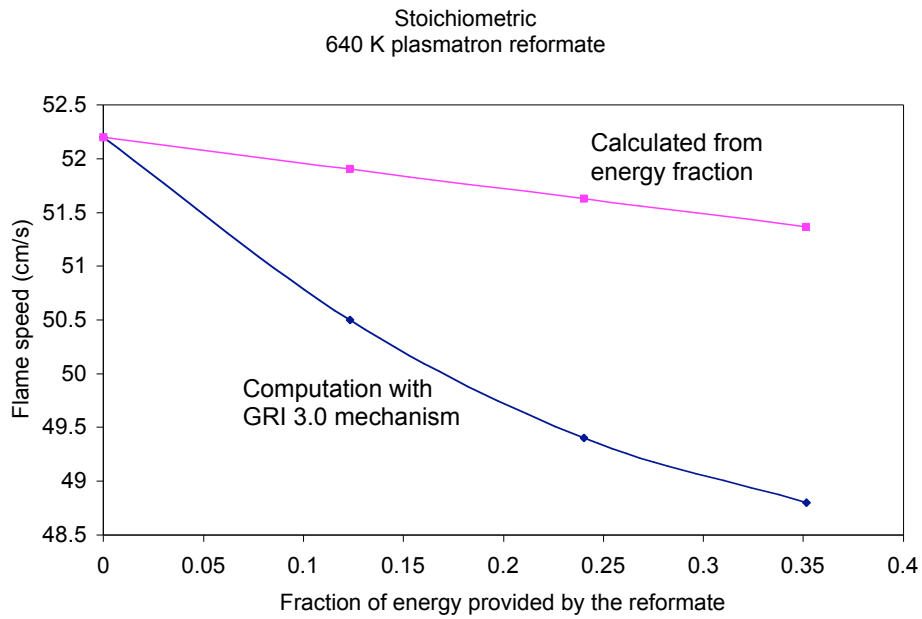
Figure 9. Laminar flame propagation speed for the conditions in Figure 8.

8 Laminar flame speed with plasmatron reformate: lean combustion

The effect of lean operation on the laminar flame propagation speed is discussed next. Explanations of effect of hydrogen enhanced engines are based upon the assumption that hydrogen rich gas increases the in-cylinder flame speed. Engine operation with engine-out emissions low enough that catalysts are not needed requires air/fuel ratios of $\lambda \sim 2$ [1,3,4,9,13-16]. Thus, this value of oxygen enrichment was chosen as illustrative in this section. The composition of the air/fuel mixture is such that the oxygen excess is 2 if all the fuel (methane and reformate) are combusted. Because the reformate carries nitrogen with it (and has, in fact, combusted some of the oxygen), it is not the air but the free oxygen that is used in the definition of lambda and its inverse, the equivalence ratio. In this section, we use $\phi_{exhaust}$. The difficulty in the definition of the equivalence ratio arises when the fuel contains substantial amounts of bound oxygen and additional nitrogen diluent, as discussed in section 4. An alternate method would use ϕ_m (from section 4) which does not includes all the oxygen used in the reforming of the fraction of the fuel. In the remaining of this paper, $\lambda = 1/\phi_{exhaust}$.

As in the case of stoichiometric combustion, the parameter that is measured to indicate the amount of reformate is the fraction of the combusted oxygen that is combusted by the reformate, called $F_{reformate}$. Table 2 shows the results for the laminar flame propagation speed as a function of $F_{reformate}$, for $\lambda = 2$. The difference in flame speeds for conditions without reformate to 30% of oxygen consumed by reformate is very small, about 2%. In other words, addition of reformate produced by the simple (uncatalized) plasmatron gasoline reformer does not affect the laminar flame propagation speed, and thus may not improve in-cylinder combustion stability.

Table 2.
Laminar flame propagation speed (v_flame)for λ =2 for different additions of reformate
(from no reformate to 15% of free oxygen combusted by reformate)

F_reformate	v_flame
	cm/s
0	9.8
0.1	10
0.2	10
0.3	10

The next case analyzed is when the reformate is not cooled. The same reformate composition as described above for gasoline is used, with the experimentally measured temperature of about 900°C (1173 K). The process to calculate the temperature of the mixture is to assume that the air/methane mixture is at 375 K, the reformate is at 1173 K. The two flows are mixed adiabatically, and then resulting temperature is increased by a factor of 1.7 (assuming $\gamma \sim 1.3$) to calculate the temperature at spark-timing. The addition of the hydrogen rich gas does not change substantially the value of γ. The resulting temperatures (T_mixture is the in-cylinder temperature at the time of inlet valve closing and T_sparking the temperature at sparking) are shown in Table 3.

Table 3
Effect of reformate addition to the temperature of air/methane/reformate mixture at IVC
(T_mixture), Temperature at sparking (T_sparking), Flame temperature (T_flame) and
$\phi_{exhaust}$ for $\lambda = 1/\phi_{exhaust} == 2$

F_reformate	0	0.1	0.2	0.3
T_mixture	375	411	445	476
T_sparking	637	699	756	810
T_flame	1750	1790	1832	1870
ϕ_m	0.50	0.51	0.53	0.54

The flame speed is shown in Figure 9 as a function of $F_{reformate}$. As opposed to the case of cool reformate, shown in Table 2, there is a large increase in the laminar flame propagation speed by the addition of the hot reformate, much larger than through the addition of even pure hydrogen (shown in Figure 5). Speeds comparable to those of stoichiometric combustion can be achieved with $F_{reformate} \sim 30\%$. The drawback of this approach is shown in Table 3, which shows the flame temperature. while it has gone up, it has not gone up to those values of stoichiometric combustion. It is not clear what effect the increase the temperature has on the generation of NOx.

Table 3 also shows the equivalence ratio ϕ_m, as defined in section 3. The oxygen required for full combustion of all the carbon and hydrogen is calculated, and then divided by all the oxygen in the air/fuel mixture. For the case when $F_{reformate} = 0$, there is no oxygen in the fuel (there is no reformate), and thus both methods of calculating the equivalence ratios agree. For higher values of $F_{reformate}$, the two methods disagree, and the equivalence ratio calculated using all the oxygen is 0.54 for the case of $F_{reformate} = 30\%$.

The effect of increased temperature from the hot reformate can be minimized by further increasing the dilution. Larger dilutions (larger than $\lambda \sim 2$) will be calculated below.
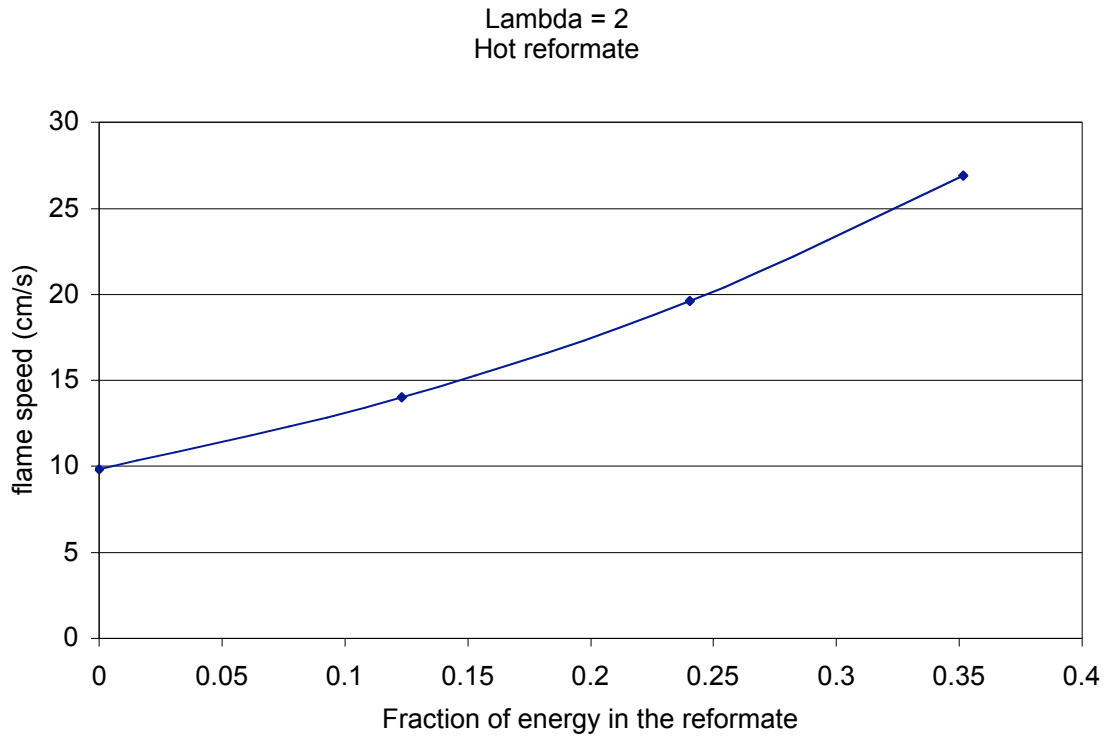
Figure 11. Laminar flame propagation speed as a function of F_reformate (the fraction of the combusted oxygen that is combusted by the reformate) for λ =2 and hot reformate.

Table 4.
Effect on flame temperature of increase F_reformate and λ at near constant flame speed

λ		2	2.2	2.4
F_reformate		0.2	0.3	0.4
T_mixture	K	445	469	487
T_sparking	K	756	797	828
φ_m		0.53	0.50	0.47
v	cm/s	19.6	19.1	18.4
T_Flame	K	1832	1782	1740

The dependence of the flame temperature on λ and on $F_{reformate}$ is shown in Table 4. In this table, the flame speed has been held approximately constant at ~ 19 cm/s, while the value of λ and $F_{reformate}$ has been varied. As λ and $F_{reformate}$ increase, the initial temperature of the air/fuel mixture and at sparking increase from 445 to 487 K and from 755 to 830 K. However, the temperature of the flame decreases, from 1830 to 1740K. This last flame temperature is comparable to that of natural gas alone, naturally aspirated, operating at λ = 2 without the addition of reformate and with a flame propagating speed of 10 cm/s (Table 3).

The final aspect that needs to be investigated is the performance with a reformate that does not include metallic plates or other heterogeneous reaction, but exclusively homogeneous. This will be done below.

The composition from the plasmatron fuel reformer when operating homogeneously without any material in the reaction s shown in Table 5.

Table 5.
Composition of homogeneous plasmatron reformate

H2	7.6%
CO	13.2%
CO2	4.8%
N2	60.8%
CH4	3.6%
C2H4	3.2%
C2H2	0.0%
O2	0.0%
H2O	6.8%

The hydrogen yield is reduced, and substantial concentrations of C_2's and methane are obtained, as well as water and CO_2.

The results from the flame speed model using the reformate composition indicated in Table 5 is shown in Table 6. Table shows the results for both the cases of hot reformate (at 1173 K) and cold reformate (at 375 K). The effect of the cold reformate on the flame speed is comparable to the reformate with the plates, shown in Table 2: the flame speed does not vary. However, when the hot reformate is used, the increase in flame speed is comparable (actually, slightly higher) than that of the reformate from the plasmatron using the plates. The increase in flame temperature is comparable for both reformate compositions. Thus, the important effect is the thermal addition, rather than the hydrogen addition.

Table 6
Impact of reformate from homogeneous plasmatron fuel converter [21]
for both hot and cold reformate addition to air/methane mixture

		No reformate	Hot reformate		Cold reformate
λ		2	2	2	2
F_reformate		0.0	0.2	0.4	0.2
T_mixture	K	375	439	496	375
T_TDC	K	638	747	843	638
φ_m		0.50	0.53	0.55	0.53
v	cm/s	9.8	18.0	30.3	9.7
T_Flame	K	1750	1814	1874	1722

9 Preignition considerations

The use of hot reformate is attractive at low to middle torque applications, including idle. It has been established that cold hydrogen rich gas is useful for preventing knock [17]. In this section, some preliminary estimates of the effect on knock of hot hydrogen rich gas addition are presented.

Calculations are performed using the engine model of CHEMKIN release 4.0.2. A Primary Reference Fuel (PRF) mechanism was used in the calculations. Gasoline is modeled as PRF with 87 octane. It was assumed that end gas is compressed by a compression ratio of 21, which represents the end gas conditions for an engine with a physical compression ratio of 10. The chemistry is followed to the point of highest compression of the end gas (corresponding to top-dead-center in the model). It is considered that if the temperature of the gas exceeds ~1200 K, the mixture is on the verge of knocking. In the absence of chemistry, the peak temperature is ~ 900K, and thus combustion of the fuel has increased the gas temperature by about 300 K. The results are not very sensitive to this choice, as once the mixture is close to knock, slight changes of the inputs will case the air/fuel temperature to increase to ~2400 K.

A limited set of calculations has been performed to determine the knock characteristics of PRF/hydrogen rich gas mixtures, at near idle conditions (1000 rpm). The calculations have been performed for two temperatures of the reformate: 900 C (1173 K), assuming no cooling of the reformate; and 375 K, assuming that the reformate does not change the in-cylinder air temperature. The reformate is mixed adiabatically with the air. The starting temperature (at IVC) of the calculations is T_mixture. It is assumed that the inlet valve closes at BDC.

Also, knock calculations were performed for two values of $\phi_m = 0.5$ ($\lambda_m = 2$), and $\phi = 1$ ($\lambda = 1$). The inlet pressure (corresponding to the pressure at IVC) is varied at constant composition and T_mixture, until the knocking conditions are determined.

Table 7
Knock-limiting pressure as a function of (a) T_mixture, for (b) stoichiometric and lean mixures

(a)

equivalence ratio, ϕm		1	1	1
T_mixture	(K)	375	385	395
knock pressure	(bar absolute)	1.05	0.93	0.79

(b)

equivalence ratio, ϕm		1	0.5
T_mixture	(K)	375	375
knock pressure	(bar absolute)	1.05	0.88

Results are shown in Tables 7 to 8. Table 7 shows the baseline case, with no reformate addition. 87 octane PRF is used without hydrogen rich gas addition. Table 7(a) shows the limiting inlet manifold pressure that avoids knock as a function of the inlet manifold temperature. There is a large effect on the knock propensity, as a 20 C increase in the inlet temperature decreases the allowable inlet manifold pressure by about 0.26 bar.

Table 7(b) shows the results for 375 K inlet manifold temperature, for two values of ϕ_m. It is interested to note that lean operation does not increase the knock-free pressure, it actually decreases the allowable pressure. This is in contrast with the results for Stokes *et al.* [22] and Topinka [17]. It is not clear the reason for the difference, and it could be due to an inappropriate chemical kinetics mechanism used in the model, or a the fact that in the experiments it is difficult to determine the actual temperature of the gas at IVC. A decrease of the temperature, either due to the injection of cold gas or more aggressive cooling with the use of a turbocharger/intercooler configuration, could mask the change due to the lean operation. Another possible explanation is that when operated lean, the exhaust temperature is cooler, and thus the temperature of the residual gases in the cylinder are lower, and thus the in-cylinder temperature at IVC would be lower. Thus, the calculations indicate that extreme care must be undertaken in analyzing experimental results, as the temperature of the initial gas is difficult to measure/control and has a large impact on the knocking propensity (in some cases, larger than the effect being investigated).

Table 8.
Knock-free pressure for no reformate, cold reformate and hot reformate, for different grades of hydrogen rich gas

Homogeneous reformate			
equivalence ratio, ϕ_m	0.5	0.5	0.5
Temperature (K)	375	375	424
Reformate	0%	20%	20%
knock pressure	0.88	0.8	0.1
Plate reformate			
equivalence ratio, ϕ_m	0.5	0.5	0.5
Temperature (K)	375	375	425
Reformate	0%	20%	20%
knock pressure	0.88	0.8	0.08
Ideal reformate			
equivalence ratio, ϕ_m	0.5	0.5	0.5
Temperature (K)	375	375	422.6
Reformate	0%	20%	20%
knock pressure	0.88	0.75	0.07

Finally, table 8 shows the knock-limiting pressure in the case of lean operation, with hot and cold reformate, for various grades of reformate. The homogenous reformate refers to the hydrogen rich generated by plasmatron reformers operating without a catalyst, with

gas composition as in Table 5. Plate reformate refers to the hydrogen rich gas composition of Table 1. Finally, ideal reformate has a composition of 28% H_2, 25% CO, balance N_2 (assuming ideal partial oxidation reforming of 87 octane PRF gasoline).

The results are surprising. Addition of all types of hydrogen rich gas actually decreases the knock-limiting pressure, even when the hydrogen rich gas is introduced cold. If the hydrogen rich gas is introduced hot, there is a large drop of allowable pressure, to torques that are actually of no interest (below 0.1 bar absolute). In addition, the ideal reformate had knock-limiting pressures lower than the results from the other hydrogen rich gas compositions, both using cold reformate and hot reformate.

These surprising results, if proven correct, indicate that the introduction of hydrogen rich gas is best when it is strongly stratified, located in the region close to the spark, with little hydrogen in the region away from it, and in particular, in the end-gas region. Strong stratification of the hydrogen rich gas should thus be investigated.

It is possible that when introducing hydrogen rich gas simulant in engine/vehicle experiments, the hydrogen rich gas is unusually cold. These experiments are not directly relevant to cases with a reformer, that produces temperatures that are substantially higher than the ambient gas temperature.

It is possible that the chemical kinetics mechanism does not include the right chemistry, and result in trends that are different from real fuels. This condition could exist even if the mechanism more or less simulates the experiments in the absence of reformate. One likely culprit, if the calculations prove wrong, is inappropriate CO chemistry.

10 Summary

For stoichiometric engine operation, pure hydrogen addition increases the in-cylinder laminar propagation speed of methane by ~20%. Ideal reformate (hydrogen, CO and nitrogen) increases the flame speed less than pure hydrogen, and reformate from homogeneous plasmatron fuel reformer does not change it at all. However, by injecting hot reformate, the in-cylinder laminar flame propagation speeds at $\lambda \sim 2$ and higher can be increased to values about half those of stoichiometric operation, at the cost of increased flame temperature (and probably increased NOx emissions). It is possible to decrease the flame temperature (and likely the peak temperature of combustion) while maintaining constant the flame speed, by increasing the fraction of the fuel that is reformed as λ is further increased.

It has been determined that the impact on the laminar flame propagation speed is due to the enthalpy addition to the air/fuel mixture from the hydrogen rich gas rather than from the addition of hydrogen. The effect of the quality of the reformate has also been calculated, and the surprising result that the hydrogen yield is not very important. However, minimization of the water and carbon monoxide in the reformate is important.

A simple formula (inverse speed-energy weighed) has been shown to be quantitatively correct to determine the laminar flame propagation speed of fuel mixtures.

Although the effects have been investigated for methane (because of limitations in the code used), the effects are likely to carry over to gasoline.

The effect of loss of volumetric efficiency can be avoided by using stratified hydrogen injection in the cylinder, or by heavier turbocharging.

However, simple knocking calculations to evaluate the effect of hydrogen rich gas addition, indicate that the different grades of hydrogen addition actually degrade the knocking characteristics of the fuel, even when the hydrogen rich gas is injected cold. Hot hydrogen rich gas addition dramatically reduces the allowable pressure in the inlet manifold.

The temperature effect has been shown to be larger than the quality of the hydrogen rich gas, both for laminar flame propagation speed (which is associated with stability), and with knock. Thus, the results indicate that extreme caution should be taken when evaluating knocking conditions or misfire when adding hydrogen rich gas. Also, if injecting hot hydrogen rich gas, it is very important for the hot hydrogen rich gas to be stratified near the location of the spark plug, with little hot hydrogen in the regions of the end gas. This sort of stratification can be easily achieved by thermal stratification by swirl flows in the cylinder, as even modest swirls results in large acceleration forces that can be effectively used for thermal stratification (hotter, less dense gas moves to the swirl axis, while colder, denser gas moves to the periphery, the region of the end gas).

Acknowledgements

References

[1] R. F. Stebar, F. B. Parks, *Emission control with lean operation using hydrogen-supplemented fuel*, SAE paper 740187 (1974)

[2] Houseman, J., and Cerini, D. J., *On-Board Hydrogen Generator for a Partial Hydrogen Injection Internal Combustion Engine*, SAE paper 740600, 1974.

[3] J. Scott MacDonald, *Evaluation of the hydrogen-supplemented fuel concept with an experimental multicylinder engine*, SAE paper 760101, 1976

[4] Jamal, Y.; and Wyszynski, M. L. *On-Board Generation of Hydrogen-Rich Gaseous Fuels: A Review, International Journal of Hydrogen Energy*, Vol. 19, No. 7, pp. 557-572, Elsevier Science, 1994.

[5] L. Bromberg, A. Rabinovich and D.R. Cohn, *Plasma Reformer/Fuel Cell Systems for Decentralized Energy Applications, International Journal of Hydrogen Energy* 22 83 (1997)

[6] D.R. Cohn, A. Rabinovich, P. Titus, L. Bromberg, *Near-term possibilities for extremely low emission vehicles using onboard plasmatron generation of hydrogen, International Journal of Hydrogen Energy* 22 715 (1997)

[7] L. Bromberg, D.R. Cohn, A. Rabinovich, J.E. Surma and J. Virden, *Compact Plasmatron Boosted Hydrogen Generation Technology for Vehicular Applications, Int. Journal of Hydrogen Energy*, 24, 341-350 (1999)

[8] John E. Kirwan, Ather A. Quader and M. James Grieve, *Advanced Engine Management Using On-Board Gasoline Partial Oxidation Reforming for Meeting Super-ULEV (SULEV) Emissions Standards,* 1999-01-2927

[9] J.B. Green, L. Bromberg, D. R. Cohn. A., N. Domingo, J.M. Storey, R.M. Wagner, J.S Armfield, *Experimental Evaluation of SI Engine Operation Supplemented by Hydrogen Rich Gas from a Compact Plasma Boosted Reformer*, SAE 2000-01-2206

[10] L. Bromberg, D.R. Cohn, A. Rabinovich and J. Heywood, *Emissions Reductions Using Hydrogen from Plasmatron Fuel Converters*, presented at Diesel Engine Emission Reduction (DEER-2000) Workshop (August 20–24, 2000, San Diego, CA)

[11] L. Bromberg, D.R. Cohn, A. Rabinovich, *Aftertreatment of Diesel Vehicle Emissions Using Compact Plasmatron Fuel Converter-Catalyst Systems, Int. Journal of Vehicle Desig*n 25, n 4, p 275-282 (2001)

[12] L. Bromberg, D.R. Cohn, A. Rabinovich, J. Heywood, *Emissions reductions using hydrogen from plasmatron fuel converters, Int. Journal of Hydrogen Energy*, v 26, 1115-21 (2001)

[13] John E. Kirwan, Ather A. Quader and M. James Grieve, *Fast Start-Up On-Board Gasoline Reformer for Near Zero Emissions in Spark-Ignition Engines*, SAE paper 2002-01-1011, 2002

[14] E. Thully and J.B. Heywood, *Lean-burn characteristics of a gasoline engine enriched with hydrogen from a plasmatron fuel reformer*, SAE paper 2003-01-0630

[15] J.A. Goldwitz and J.B. Heywood, *Combustion Optimization in a Hydrogen-Enhanced Lean Burn SI Engine*; SAE paper 2005-01-0251

[16] Z. Ivani, F.Ayala, J.A.Goldwitz, J.B. Heywood, *Effects of Hydrogen Enhancement on Efficiency and NOx Emissions of Lean and EGR-Diluted Mixtures in a SI Engine*, SAE paper 2005-01-0253

[17] J.A. Topinka, M.D. Gerty, J.B. Heywood, J.C. Keck, *Knock behavior of a lean-burn, H_2 and CO-enhanced, SI gasoline engine concept,* SAE paper 2004-01-0975

[18] Y. Huang, C.J. Sung, J.A. Eng, *Laminar flame speeds of primary reference fuels and reformer gas mixtures*, Combustion and Flame **139**, n 3, November, 2004, p 239-251

[19] R. J. Kee, F. M. Rupley, J. A. Miller, M. E. Coltrin, J. F. Grcar, E. Meeks, H. K. Moffat, A. E. Lutz, G. Dixon-Lewis, M. D. Smooke, J. Warnatz, G. H. Evans, R. S. Larson, R. E. Mitchell, L. R. Petzold, W. C. Reynolds, M. Caracotsios, W. E. Stewart, P. Glarborg, C. Wang, O. Adigun, W. G. Houf, C. P. Chou, S. F. Miller, P. Ho, and D. J. Young, CHEMKIN Release 4.0, Reaction Design, Inc., San Diego, CA (2004).

[20] G.P. Smith, D.M. Golden, M. Frenklach, N.W. Moriarty, B.Eiteneer, M. Goldenberg, C.T. Bowman, R.K. Hanson, S. Song, W.C. Gardiner, Jr., V.V. Lissianski, and Z. Qin, *GRI 3.0 mechanism*, *http://www.me.berkeley.edu/gri_mech*/

[21] L. Bromberg, D.R. Cohn, K. Hadidi, J.B. Heywood, A. Rabinovich, *Plasmatron Fuel Reformer Development And Internal Combustion Engine Vehicle Applications*, Presented at the Diesel Engine Emission Reduction (DEER) Workshop, 2004 Coronado CA, August 29-September 2, 2004

[22] J. Stokes, T. H. Lake and R. J. Osborne, *A Gasoline Engine Concept for Improved Fuel Economy –The Lean Boost System*, SAE paper 2000-01-2902