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ABSTRACT
The use of hydrogen as an engine fuel has great potential for reducing exhaust emissions with the exception of a small amount of carbon containing emissions originating from the lubricating oil, NOx is the only pollutant emitted. In this paper by using a turbulent flame speed method, a quasi-dimensional thermodynamic model of an SI engine fueled with hydrogen is developed. In this work, simulation results are validated by experimental data. Then the effect of spark advance, A/F ratio and valve timing on emission and performance characteristics of the modeled engine has been investigated. Hence, remarkable effects in emission and performance characteristics observed. And the behavior of the modeled engine against the above parameters has been investigated and the reason of that is discussed.

Keywords: A/F ratio, Emission, Hydrogen, Performance, valve timing.

INTRODUCTION
Hydrogen can be produced from many different feedstocks, including natural gas, coal, biomass, and water. If hydrogen is produced from renewable sources, the global warming potential, which nowadays is a major problem and a hot topic, of hydrogen is insignificant in comparison to hydrocarbon based fuels since combustion of hydrogen produces no carbon-based compounds such as HC, CO, and CO2 [1]. If hydrogen is produced using renewable energy, it is an energy carrier that reduces emissions of noxious exhaust gases and greenhouse gases to zero or a very small fraction of the emissions found when using traditional fossil fuels.

Hydrogen has special properties so the combustion characteristics of hydrogen are very different from gasoline. The laminar flame speed of a hydrogen air mixture at stoichiometric condition is about 10 times that of gasoline. It has a wide flammability limit, preignition and back firing can be a problem. The flammability limits correspond to equivalence ratios of 0.07 to 9 [1]. Water injection into the intake manifold is used to mitigate preignition and provide cooling. Exhaust gas recirculation and lean operation are used to reduce NOx levels. Also the octane rating of hydrogen of 106 RON [1] allows increasing compression ratio.

Hydrogen is one of the most interesting alternative fuels, and is recently in the centre of attention. Hydrogen can be produced from renewable sources and offers lots of other benefits. One of the most practical one is its ability to run in bi-fuel conditions. Also Hydrogen internal combustion engines have the ability for an increased efficiency [2].

Comprehensive overview of hydrogen engine properties and design features is already done by previous authors and it was concluded that hydrogen internal combustion engines have a high efficiency, are very clean and considerably cheaper than fuel cells [3].

Limited numbers of previous publications have worked on hydrogen engine simulation. A two-zone quasi-dimensional engine model for calculating power and NOx emission was demonstrated in Fagelson et al. publication [4]. In their work laminar burning velocity is...
calculated from a second order reaction with estimated activation energy.

In another literature [5] the same model was used in order to predict the performance of a supercharged hydrogen engine. They report an overestimation of the rate of pressure rise that can be a consequence of an overestimation in burning velocity. Another publication [6] use a Wiebe's law in a zero-dimensional model. And for a varying compression ratio and ignition timing the optimum cylinder diameter for the minimum emission and maximum power for a fixed equivalence ratio calculated.

In Verhelst's literature [7] quasi-dimensional model was preferred to multi-dimensional one because of a reasonable accuracy and fast computation on PC system. And they developed a complete cycle simulation code for SI engine and they looked thoroughly at the turbulent combustion in hydrogen fuelled engine. In another publication [8] a simulation and design tool applicable to hydrogen powered spark ignition engine systems is introduced. The code is applicable to single and multi-cylinder engines under steady state or transient operating conditions the model is validated against experimental data for the intake flow model.

In this paper, first of all a quasi-dimensional code for the four strokes of SI hydrogen engine is developed. In this simulation the turbulent flame speed is modeled based on previous literature and also some modification was applied to the flame speed method. The model then calibrated matching the data obtained in the previous experiment [9]. A combination of valve timing, spark advance (SA) and air to fuel ratios variations on engine emission and performance is also studied.

**ENGINE MODEL**

The engine model is a quasi-dimensional two-zone model which solves the basic differential equations for the intake, compression, power and exhaust strokes.

In this model, the combustion chamber is divided into two zones, which one should imagine as being divided by flame front, zone 1 contains unburned mixture and zone 2 contains burned mixture. Thermal NOx formation also takes place in burned zone, which is described by the extended Zeldovich mechanism [10]. The flame front is assumed to travel by a speed called turbulent flame speed which is a function of laminar flame speed that is computed from previous studies [11].

The engine model uses Woschni correlation [12] to estimate engine heat transfer this correlation is not accurate for hydrogen, considering the lack of any accurate validated alternative the error of the Woschni correlation for hydrogen engines is inevitably accepted in the model. Burned unburned zones are calculated by assuming that the flame travels in a sphere like shape. The engine model also includes a friction model to predict brake mean effective pressure. The frictional processes in an internal combustion engine can be categorized into three main components: (1) the mechanical friction, (2) the pumping work, and (3) the accessory work. For this work a method, which calculates the total friction work accurately, was used [1]. The applied friction model spontaneously predicts all the categories above.

The composition of the reaction products is calculated from the chemical equilibrium at a given pressure and temperature of the 12 species \( N_2, NO, N, CO_2, CO, OH, H, O_2, O, H_2O, H_2, Ar \). An optimization calculation procedure is used to calculate the mole fraction of each species and the total mole fraction [13].

The engine model is validated by comparing the simulated result with the experimental data taken from a previous engine experiment [9]. The engine used in the experimental evaluation is a dedicated hydrogen-fueled engine. The dedicated hydrogen-fueled engine is the descendant of a gasoline-fueled engine, which was later converted to hydrogen-fueled one.

**LAMINAR FLAME SPEED** - Flame speed is a critical effective parameter in model results, so using an accurate formulation is essential. Almost all of the turbulent combustion models assume that the combustion happens in flamelet regime. It is then assumed to travel locally at the laminar flame speed, therefore it is necessary to know the laminar flame speed of the hydrogen/air mixture. First a short overview over hydrogen burning velocity is given.

Liu and MacFarlane – In their publication [14] laminar burning velocity of hydrogen/air mixture was measured and their measurements resulted in a formula as a function of fuel/air equivalence ratio and residual gas mole fraction.

Milton and Keck – Milton and Keck [15] took out the laminar burning velocity of stoichiometric hydrogen/air mixture from some experiments. Then they fitted a correlation to the experimental data.

Ijima and Takeno - Ijima and Takeno [11] described the laminar burning velocity of hydrogen/air mixture by a zero-dimensional analysis. Their experiments resulted in a formula which will be shown.

Other Kinds of formula has been developed by some other authors too, including Koroll, Kumar and Bowels [16], Taylor et al. [17], Law et al [18], Kobayashi et al [19]. All of the above formula can be seen in their publications.

From all the correlations developed by the authors above only Iijima and Takeno’s [11] formula is a function of the three of the fuel/air equivalence ratio, temperature and pressure. The other’s formulation doesn’t include one of them so their equation has the enough integrity.
that was needed for this work. Iljima and Takeno’s correlation is not a function of residual gas, therefore in this paper their correlation is modified by a residual gas effect term which is taken from Verhelst’s correlation [20]. Iljima and Takeno’s [11] formula is as follows:

\[ u_1 = u_{10} \left( \frac{T_u}{T_0} \right)^{\alpha_T} \left[ 1 + \beta_p \log \frac{P}{P_0} \right] \]  

Flame speed is in (m/s).

The modified correlation is:

\[ u_1 = u_{10} \left( \frac{T_u}{T_0} \right)^{\alpha_T} \left[ 1 + \beta_p \log \frac{P}{P_0} \right] (1 - \gamma f) \]  

Where: \( P \) is the pressure, \( T_u \) is the unburned temperature, \( f \) is the residual gas volume fraction, \( T_0=291(K), P_0=101325(Pa) \).

\( \alpha_T \) and \( \beta_p \) are as follows:

\[ \alpha_T = 1.54 + 0.026 (\phi - 1) \]
\[ \beta_p = 0.43 + 0.003 (\phi - 1) \]  

Where, \( \phi \) is the fuel air equivalence ratio. The parameter \( \gamma \) expressing the effect of residual gases is given by:

\[ \gamma = 2.715 - 0.5\phi \]  

And \( u_{10} \) which is the laminar burning velocity of hydrogen at 291(K) and 1(atm), in (m/s), given by:

\[ u_{10} = 2.98 - (\phi - 1)^2 + 0.32 (\phi - 1.70)^3 \]  

By using the above values the simulation results was accurate for different engine speed and conditions. It should be considered that the method above does not produce a stable and stretch-free laminar burning velocity.

TURBULENT FLAME SPEED – Many methods for describing and calculating the turbulent flame speed have been developed by previous authors. In this paper the so-called “Damkohler and derivatives” method [20] is used according to this model turbulent flame speed is as follows:

\[ u_t = u'_{TDC} (1 - 0.5 \frac{\theta - 360}{45}) \]
\[ u'_{TDC} = 0.75U_p \]

\( \theta \) is the crank angle (360 at TDC of compression).

The above correlation has been validated for specific engine geometry. In this paper the method above was calibrated by some calibration factors to fit the current engine geometry and hence producing accurate results.

MODEL VALIDATION

The engine used is a dedicated hydrogen-fueled engine which was converted from a gasoline engine to bi-fuel operation and later used when operated by hydrogen.

By using the modified Iljima and Takeno method a two zone engine model in Matlab environment is developed. Engine specification, which can be observed in Table 1, was imported to the model. The calculated data was validated by previous experimental work [9]. The calculated and experimental in cylinder pressure versus the crank angle is really near to each other, which can be observed in Fig1. This shows that, using the modified Iljima and Takeno flame speed method was suitable.

The fuel air ratio for Fig1 is not a practical one but only on this particular condition, P-theta diagram was presented in the related literature [9] so this was used for validation inevitably.

### Table 1 Engine specification

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement</td>
<td>430.8 cc</td>
</tr>
<tr>
<td>Bore</td>
<td>86.0 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>74.2 mm</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>9.7</td>
</tr>
<tr>
<td>Intake valve diameter</td>
<td>36.0 mm</td>
</tr>
<tr>
<td>Exhaust valve diameter</td>
<td>25.4 mm</td>
</tr>
<tr>
<td>Intake valve lift</td>
<td>8.4 mm</td>
</tr>
<tr>
<td>Exhaust valve lift</td>
<td>5.7 mm</td>
</tr>
</tbody>
</table>
The results for the experimental and simulated NOx concentration, which is calculated from extended Zeldovich mechanism [10], versus equivalence fuel/air ratio for some points, can be seen in Fig.2. As it is seen that the simulated and experimental results for NOx concentration is pretty good for low fuel air equivalence ratio but the model under-predicts NOx concentration at high fuel air equivalence ratio, which is not a practical operating condition. And this difference from experiment can be probably because of the error of using Woschni’s heat transfer correlation and the error of the flame speed correlation used. As this error occurs in a non practical operating condition, it can be neglected. Also the experimental and calculated results for BMEP versus fuel/air equivalence ratio is shown in Fig.3. The results are near enough with a little difference which can be a result of heat transfer and flame speed correlations error, this shows that the engine model works good enough.

**AIR TO FUEL RATIO**

A/F ratio plays a very important role in engine performance and emissions characteristics. Hydrogen has special properties so the combustion characteristics of hydrogen are very different from gasoline. The laminar flame speed of a hydrogen air mixture at stoichiometric condition is about 10 times that of gasoline. The wide flammability limit of hydrogen allows the use of very lean fuel/air equivalence ratios, as low as 0.2, which result in reducing NOx emissions.
The major effect of A/F ratio on engine NOx emission for different engine speeds is shown in Fig.4. As it is shown the value of NOx emission is varied from 16000 (ppm) to near zero respecting to fuel/air equivalence ratio. Maximum amount of NOx emission occurs when the fuel/air equivalence ratio is about 0.8 and this happens in a wide range of engine speeds. As it is shown in Fig.4 the NOx concentration peak at near 0.8 fuel/air equivalence ratio, but as the mixture becomes leaner the NOx concentration falls dramatically. One of the most important parameter in determining SI engine emissions is the fuel/air equivalence ratio and in hydrogen engines it is much more important and controlling this parameter is really important and effective.

A/F ratio has a major effect on IMEP. This effect is shown on Fig.5. As it is shown the value of IMEP is varied from near 4 to near 10 bar respecting to fuel/air equivalence ratio. Maximum amount of IMEP occurs when the fuel/air equivalence ratio is about 1, stoichiometric condition, and this repeats in a wide range of engine speeds.

**SPARK ADVANCE**

Spark advance (SA) is another parameter that has a major effect on engine performance and emission. Fig.6 shows the IMEP versus spark advance (SA) for different engine speeds. As it is seen in low engine speeds, 1000-1800 (rpm), the maximum IMEP happens when the spark advance range is [-5 0]. But as the engine speed increases the maximum IMEP happens in more advanced spark and in 4000 (rpm) this point is near 20 degrees before TDC.

Spark timing significantly affects NOx emission levels. Advancing the timing so that combustion occurs earlier in the cycle increases the peak cylinder pressure, retarding the timing decreases the peak cylinder pressure.

Higher peak cylinder pressures result in higher peak burned gas temperatures, and hence higher NOx formation rates. For lower peak cylinder pressures, lower NOx formation rates result [10].

This matter is shown on Fig.7 and it can be seen that the NOx varies between about 600 (ppm) to near zero respectively to spark advance. This shows the major importance of spark advance on hydrogen engine's characteristics.
VALVE TIMING

In internal combustion engine valves behavior (lift and timing) is one of the most important parameters which have a major effect on the engine operation and emission. By using VVT technology we are able to control engine behavior in any conditions with the purpose of decreasing emission and optimizing engine operating characteristics.

As it is shown on Fig.8 as the IVO advances NOx concentration and IMEP increases due to volumetric efficiency increase, and consequently increase of in-cylinder temperature but when the volumetric efficiency approaches its maximum the valves overlap effect shows up. Valves overlap factor increase the amount of residual gas. Any burned gas in the unburned mixture reduces the heating value per unit mass of mixture and, thus, reduce the adiabatic flame temperature [10]. Therefore as the residual gas mass fraction increases, IMEP decreases and as a result of reduction of in-cylinder temperature, NOx concentration falls.

As the EVO advances the exhaust valve opens in higher in-cylinder pressure therefore more burned gas leaves the cylinder and there is less residual gas so the NOx concentration and IMEP increase because more fresh mixture enters the cylinder but as the EVO advances more and more in one point the valves overlap factor overcomes the first effect and therefore residual gas increases and this causes an decrease in NOx and IMEP. These trends can be seen on Fig.9.

One of the other effective variables which can be controlled by using VVT mechanism is valves (Intake and exhaust) lift. By increasing the intake valve lift the volumetric efficiency and therefore in-cylinder temperature increases and this cause an increase in IMEP and NOx concentration, intake valve lift increase also causes an increase in valves overlap factor so as the intake valve lift increases the valves overlap effect causes an increase in residual gas and therefore decrease in NOx concentration, the trends mentioned can be seen on Fig.10.
As the exhaust valve lift increases more burned gas leave the cylinder and therefore there is less residual gas in the cylinder and this causes an increase in NOx concentration, as it is shown in Fig. 11, as the residual gas decreases more fresh mixture enters the cylinder and IMEP increases.

Valves opening duration which is the time between valves (intake or exhaust) opening till closing can be controlled by using VVT mechanism at different conditions.

When the intake valve opening duration increases volumetric efficiency increases too and this cause a rise of in-cylinder temperature and consequently NOx concentration grows. But when the duration increases more and more valves overlap factor increases too and therefore residual gas grows and eventually NOx concentration reduces.

The mentioned series of events also affects the IMEP. By increasing the intake valve opening duration, IMEP increases and by further increase in duration, IMEP declines because of an increase in residual gas mass fraction.

As the exhaust valve opening duration increases more burned gas leaves the cylinder so more fresh mixture fills the cylinder in the intake stroke this cause a sharp increase in IMEP and in-cylinder temperature.

Therefore, as it is shown on Fig. 13 NOx concentration rises too. By increasing duration more, the overlap factor increases and consequently residual gas increases, so the NOx concentration and IMEP falls slightly.

**CONCLUSION**

The purpose of this work was to develop a hydrogen engine model which can be used as an engine simulator.
to predict engine emission and performance characteristics with accurate results. The engine simulator was validated by experimental data.

In this paper also sensitivity of hydrogen engine to spark advance, A/F ratio and valve timing studied and their importance were shown. It was shown that the hydrogen engine has its most NOx concentration at the point near to \( \phi = 0.8 \). Also SA effect was studied and the major effect of this parameter considered and discussed. Variation of valves lift, opening time and duration was studied and the reason of their effects fully discussed. The valve timing studies can also be applied to VVT mechanism.

REFERENCES


ADDITIONAL SOURCES

DEFINITIONS, ACRONYMS, ABBREVIATIONS

A/F: Air to fuel
atm: atmosphere
BMEP: Brake mean effective pressure
BTDC: Before top dead centre
CA, θ: Crank angle
CI: Compression ignition
EVO: Exhaust valve opening
f: Residual gas volume fraction
IMEP: Indicated mean effective pressure
IVO: Intake valve opening
MBT: Maximum brake torque
NOx: Oxides of nitrogen
P: Pressure
ppm: Parts per million
RON: Research octane number
rpm: revolution per minute

SA: Spark advance
SI: Spark ignition
T: Temperature
TDC: Top dead centre
u': Root mean square turbulent velocity
U_p: Mean piston speed
α_T: Temperature exponent
β_P: Pressure exponent
γ: Residual gas coefficient
φ: Fuel to air equivalence ratio
VVT: Variable valve timing

Subscripts:
0: Reference condition
t: turbulent
u: Unburned