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Simulation of Engine Combustion with Ethanol as a Renewable Fuel

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ABSTRACT:
Ethanol as a fuel is an important bio-fuel for future energy needs. In this work the combustion process of gasoline-ethanol blends in spark ignition engines was investigated using computational fluid dynamics and turbulent combustion modeling. A modified flame surface density approach developed for gasoline engine combustion was adapted to calculate fuel-burning rate of the blend. The rise in in-cylinder peak pressure and temperature for blends up to E20 was found relatively small compared to E00. A significant reduction of CO and an increment of NOx were observed for optimized combustion with adjusted ignition timing.

Key words: ethanol, combustion, simulation, engine

I. Introduction

More recently, the increasing oil prices, depletion of oil reserves and political instabilities in oil rich countries have highlighted the need to reduce the dependency on petroleum-based oils. Thus as a promising alternative bio fuel, ethanol has drawn some attention [1-2]. Invention of novel methodologies to extract bio ethanol from second-generation feed-stocks has made the use of ethanol more attractive and more sustainable.

According to experimental findings, ethanol exhibits similar combustion characteristics as gasoline. Ethanol and gasoline can be used as a blend in conventional Spark Ignition (SI) engines. Interestingly, small blending proportions of ethanol can easily be used in existing engines without any engine modifications. Ethanol blending results in better anti-knock characteristics due to higher octave number in ethanol [2]. Also, usually it makes the combustion much cleaner with higher power and less hydrocarbon emissions. However, as a result of higher burning temperatures NOx increases. Even though it is possible to run SI engines on 100% (E100) ethanol, its worldwide use is prohibitive mainly due to the fact that the present engine technology is not yet advanced enough to extract the full potential from E100 combustion. In this regard, combustion modelling integrated with Computational Fluid Dynamics (CFD) can be used as an effective tool to understand ethanol combustion characteristics in engines and to develop advanced IC engine technologies for ethanol use.

This paper demonstrates the capability of CFD and turbulent combustion modelling for the prediction of combustion characteristics of gasoline ethanol blends in SI engine applications. By the incorporation of CFD with advanced combustion models, combustion characteristics of a number of ethanol gasoline blends ranging from E00 to E20, are simulated using a newly formulated Bray-Moss-Libby [3] type turbulent combustion model. The model was originally developed and validated for gasoline combustion and extended here to predict the burning rates of anhydrous gasohol blends. Modifications required in engine operating conditions, such as spark timing, to optimise the combustion is examined and potential gain in power is also analysed. Effect of ethanol addition on exhaust emission formation is also investigated.

II. Computational Modelling Approach

In this study CFD modelling is used to conduct full cycle engine simulations of a Ricardo E6 port fuel injected, SI engine running with different ethanol mixtures. It was assumed that gasoline and ethanol blend is fully mixed in gaseous state and uniformly distributed within the engine cylinder. This is an accurate assumption for port fuel injection engines where fuel is injected during the early stage of the intake stroke so that adequate time is available for fuel evaporation and mixing. Unburned gas consumption rate \( \bar{\omega} \) was modelled using the flame surface density approach given by,

\[
\bar{\omega} = \rho_u I_0 S_1 \Sigma
\]

where, \( \Sigma \) is the flame surface density: the available flame surface area per unit volume . \( \rho_u \) is the unburned gas density and \( S_1 \) is the unstretched laminar burning velocity. The factor \( I_0 \), account for the stretch and curvature effects of flamelets on the burning velocity. \( \Sigma \) is evaluated using the following modified formulation of the BML model.

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\[ \Sigma = C_{BML} \frac{(1+2\varepsilon)}{0.7} \frac{\varepsilon(1-\varepsilon)}{1+5.715 \frac{Re}{Re_{\lambda}} + 72.051 \left( \frac{u'}{\epsilon} \right)^3} \frac{S_t}{6D-12} \]  

\[ S_t = (1 + 0.07V^{0.35})\phi^{-0.326}\exp[-4.48(\phi - 1.075)^2] \left( \frac{T}{300} \right)^{1.56+0.23V^{0.64}} \left( \frac{P}{1.6} \right)^{-0.22} (1 - f\varphi) \]

where \( T, P \) and \( V \) are the unburned gas temperature in Kelvins, in-cylinder pressure in bars and the volume fraction of ethanol in the fuel blend. \( f \) is a factor that accounts for the effects of residual gas mass fraction \( \varphi \) on the laminar burning velocity and \( \phi \) is the fuel air equivalence ratio of the fuel air mixture. The laminar flame speed \( S_t \) has the units \( \text{ms}^{-1} \). \( \phi \) is a varying function of mixture composition and defined as the ratio between required stoichiometric oxygen mass and the available oxygen mass. It should be noted here that only a very few studies have published correlations for the laminar burning speed of gasoline-ethanol blends. Among them Gulder’s [6] formulation is the only study based on a comprehensive analysis of experimental data. Ignition process and early flame kernel growth was modelled using the discrete particle ignition kernel model [7]. Chemical species formation was modelled with a simplified reaction scheme assuming single step fuel oxidation. The blend was considered to be an anhydrous mixture of iso-octane and ethanol. In addition, dissociation reactions were modelled using six reversible reactions and they were solved using the iterative equilibrium solver in KIVA4. Extended Zeldovich mechanism was used for modelling NO\textsubscript{x} formation. The reactions used are summarised in Table 1.

<table>
<thead>
<tr>
<th>Fuel oxidisation</th>
<th>Chemical equilibrium</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol: C\textsubscript{2}H\textsubscript{5}OH + 3O\textsubscript{2} \rightarrow 2CO\textsubscript{2} + 3H\textsubscript{2}O</td>
<td>H\textsubscript{2} ⇌ 2H</td>
</tr>
<tr>
<td>Iso-octane: 2 C\textsubscript{8}H\textsubscript{18} + 25 O\textsubscript{2} \rightarrow 16 CO\textsubscript{2} + 18 H\textsubscript{2}O</td>
<td>O\textsubscript{2} ⇌ 2O</td>
</tr>
<tr>
<td>Extended Zeldovich mechanism : kinetic reactions</td>
<td>N\textsubscript{2} ⇌ 2N</td>
</tr>
</tbody>
</table>

The above combustion model was first validated against the experimental data for gasoline only (E00) combustion in a Ricardo E6 engine. Subsequently, using the validated model, the combustion performance of ethanol gasoline blends up to 20% (E20) was examined. The computational mesh used in the present study contained 400,000 cell elements and is shown in Fig.1. The engine specifications and operating conditions of the engine are shown in Table 2.

III. Results and Discussion

In cylinder combustion process is largely affected by the turbulence intensity and the bulk flow pattern within the cylinder. Shown in Fig. 2(a) and 2(b) respectively are the predicted velocity magnitude field of the present test case at the end of the intake stroke and before ignition. A distinct swirl and tumble motion can be identified, which essentially enhances fuel mixing and vaporisation. Fig. 2(b) shows the turbulent kinetic energy field before the start of ignition. A relatively low level of turbulence can be noticed near the spark location, hence the turbulent effects on early flame wrinkling can be expected to be very small.
TABLE 2

<table>
<thead>
<tr>
<th>GEOMETRIC DETAILS OF RICARDO E6 ENGINE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (cm)</td>
</tr>
<tr>
<td>Stroke (cm)</td>
</tr>
<tr>
<td>Squish* (cm)</td>
</tr>
<tr>
<td>Con. Rod Length (cm)</td>
</tr>
<tr>
<td>Intake Valve Opening</td>
</tr>
<tr>
<td>Intake Valve Closing</td>
</tr>
<tr>
<td>Exhaust Valve Opening</td>
</tr>
<tr>
<td>Exhaust Valve Closing</td>
</tr>
<tr>
<td>Engine RPM</td>
</tr>
<tr>
<td>Equivalence Ratio</td>
</tr>
</tbody>
</table>

*Squish - distance between piston crown & cyl. head @ TDC

Important notes:
- Equivalence Ratio:** 0.967
- Engine RPM:** 1800

Fig. 1: Computational mesh for Ricardo E6 engine

Fig. 2. (a) Distribution of the flow velocity field at 20 CAD after the bottom dead centre in the tumble plane (b) in the swirl plane before ignition (c) Turbulent Kinetic energy profile on spark location plane at 344 CAD. (d) Predicted and measured in-cylinder pressure comparison for E00 combustion

Fig. 2(d) shows the present combustion model predictions compared with experimentally measured in-cylinder pressure values for the E00 mixture. The model has been previously validated for a range of operating conditions of the E6 engine and reported elsewhere [8] and only the results corresponding to the present test case are presented here. Model predictions during the early and middle stages are in very good agreement and the discrepancies in the latter stage are due the absence of a blow by model in the present formulation.

Fig. 3(a) and 3(b) show the predictions of the present laminar flame speed model for different mixture compositions. It is evident that the flame speed increases with the increasing ethanol fraction. However, the rate of increase appears to be nonlinear, where a large increment in flame speed can be seen for a small increase in ethanol fraction. This effect has a direct influence on the in-cylinder pressure rise as shown in Fig. 3(c). The engine spark advance here corresponds to the maximum brake torque (BMT) at 1800 rpm. The equivalence ratios of all the mixtures were considered to be 1.0 and rest of the initial conditions were kept similar to E00 simulation conditions. The results show that the peak in-cylinder pressure appears to reach a maximum with E15 and beyond E15, pressure rise reach a saturation. This observation is well in agreement with the experimentally observed trend in Baraktar [9].

Shown in Fig 4(a) is the in-cylinder instantaneous maximum temperature for different ethanol mixtures. Temperature also increases with the ethanol furcation but saturates after E15. The reason for this saturation in both temperature and pressure is that the advantage gained by increasing flame speed of gasohol blend is hindered by the low energy content of ethanol. Due to higher temperatures around 5% reduction of CO was observed. However, this reduction of CO diminishes with the increasing ethanol fraction, as the temperature increment saturates. NOx level has also been found to increase by nearly 15% at saturation level. Effect of the change in ignition timing was investigated and presented in Fig.4(c). A considerable reduction in both CO and NOx was observed when ignition
timing was retarded by three degrees. For this case, the indicated mean effective pressure (IMEP) was slightly lower compared to MBT timing of gasoline. For all the retarded ignition time cases, an increase of CO and NO\textsubscript{x} were observed while the reduction in IMEP was a minimal. These results verify that ignition timing plays a vital role for the fine-tuning of the engines operating with ethanol and gasoline blends. The optimum operating conditions are always a compromise between power and emissions.

![Figure 3: Laminar flame speed variation with (a) equivalence ratio (b) temperature. (c) The predicted in-cylinder pressure for ethanol gasoline blends.](image)

Fig. 3: Laminar flame speed variation with, (a) equivalence ratio (b) temperature. (c) The predicted in-cylinder pressure for ethanol gasoline blends.

![Figure 4: Effect of ethanol fraction on (a) Maximum in cylinder temperature and (b) Emissions. Fig. 4(c) shows the effect of spark timing on IMEP and emissions.](image)

Fig. 4: Effect of ethanol fraction on (a) Maximum in cylinder temperature and (b) Emissions. Fig. 4(c) shows the effect of spark timing on IMEP and emissions.

### IV. Conclusions

This study has demonstrated the use of CFD and combustion simulations approach for the investigation of ethanol based engine performance. A CFD engine model, validated with experimental gasoline data, has been successfully implemented to simulate engine conditions using different ethanol mixtures. Modeling results of gasoline-ethanol combustion confirmed that the existing engines should be able to run with small ethanol fractions blended with gasoline without any hardware modification, as the rise in peak pressure and temperature are very small. However, the results also show that the optimum operating conditions for gasoline ethanol blends are somewhat different from the gasoline combustion conditions. It is also shown that, small fractions of ethanol up to E10 can be added without sacrificing engine power or emissions. For an optimal operation with lower emissions, ignition timing has to be adjusted accordingly.

### References


