Numerical Modelling of Methanol-Gasoline Blends in PFI Spark Ignition Engines

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Abstract. According to present statistics, India is the 6th highest consumer of fossil fuels in the world. This raises high concerns in terms of emissions and import bills. Most recently India has taken stand to promote alternate fuels such as Methanol/biofuels and blends as substitute for conventional fuels. The use of blended fuel, without change in configuration of engine or in operating parameters can lead to lower performance. Operating parameters are to be optimized to obtain improvement in performance. Optimization requires rigorous experimentation, which increases cost of production for automotive manufacturers and simulation facilitates an early understanding of the engines behaviour. In this study, a 0.8 litre, 27.6 kW PFI engine is modelled and analysed to investigate the response of methanol-gasoline blends and experimental work is conducted for validation. Results indicated, with methanol blended up to 20% by volume, engine brake power was lower than base line gasoline but for blends of 20-50% by volume brake power and torque showed higher value than gasoline values. For M30, M40 and M50 with blend composition there was a proportionate increase in BSFC for all speed ranges.

Keywords: Alternative fuels, Engine, 1-D Simulation, Methanol blends, SI engine, Port Fuel Injection

1. Introduction

Energy scarcity is becoming a major concern around the globe. At present, major contribution of energy requirement for transportation, domestic and commercial requirement are addressed by combustion of fossil fuels. Economic considerations such as import bill, fluctuations in the price of fuel and harmful exhaust gas emissions impetuses government and automotive manufacturers to focus on alternative fuels, which are renewable to replace conventional fuels. Alcohols and alcohol based fuels were tested and used in Internal Combustion Engines (ICE) for more than a century. Earlier work on alcohol in ICE is dated to 19th century in the literature. Alcohol based fuels are classified as renewable sources and are highly regarded for reduced greenhouse gases and increased of thermal efficiency during combustion. With stringent emission norms and emphasis on improvement in efficiency more research work is carried out on alcohol fuels. Some of the most commonly preferred alcohols in ICE are ethanol, butanol, methanol, and fuselol and ethers (methyl tertiary butyl ether (MTBE) and Dimethyl Ether (DME)). Most preferred alcohol for Spark ignition (SI) engine applications have been blends of ethanol with gasoline. Presently 5-10% of ethanol in gasoline is acceptable according to fuel quality standards [1-4].
Investigations to use methanol as a substitute for gasoline to enhance engine performance were conducted during 1930s. Chemical formula of methanol is CH$_3$OH. It has a monatomic carbon per molecule, which is connected to hydrogen atoms in a single bond and there is an absence of strong carbon to carbon bond. This helps in reduction of soot and hydro-carbon emissions in IC engines. The structure of methanol is illustrated in Fig 1.1.

![Structure of Methanol](image.png)

Properties of Methanol and Gasoline are tabulated in Table 1.1. Advantages of methanol includes that it is a renewable fuel, produces low exhaust emissions and relatively low cost compared to gasoline, by the present market in India price of methanol is approximately 19-28 INR/litre while that of gasoline is 81 INR/litre. Methanol can be produced from several sources such as from hydrogen and carbon monoxide as syngas, from natural gas, gasification of coal and also through production of biomass.

| Properties                  | Methanol | Gasoline   |
|-----------------------------|----------|------------|
| Molecular formula           | CH$_3$OH | C$_8$H$_{18}$ |
| Molecular weight            | 32       | 95–120     |
| Oxygen content (%)          | 50%      | 0          |
| Density (kg/m$^3$)          | 792      | 740        |
| LHV (MJ/kg)                 | 20       | 44.3       |
| Octane number               | 111      | >90        |
| Auto-ignition temp. (°C)    | 465      | 228–470    |
| Stoichiometric A/F ratio    | 6.47     | 14.8       |
| Latent heat of vaporisation (kJ/kg) | 1103 | 305        |
| Boiling point (°C)          | 64       | 38–204     |
| Flash point (°C)            | 11       | -45        |

From present reports, India consumes close to 2900 cr litres of petrol and 9000 cr litres of diesel per year, this makes India the 6th highest consumer in the world. According to statistics, consumption is predicted to become twice of the present, and this will make India 3rd largest consumer by 2030. Present account on import bill is almost 6 lac crores. In India Ministry of Road transport & Highways passed the bill to promote methanol as indigenous fuel for transportation to address high import bills and to cut down emission rates [7].

Methanol-Gasoline blends in IC engines have un-explored potentials to improve efficiency and can play a vital role to bring down emissions. Methanol has good compatibility with various technological enablers and requires further optimizations. Experimental investigations are expensive and requires well established lab facilities but results are accurate and reliable.
Numerical methods require accurate reference data and have complex calibration & validation procedures. In Gasoline engines, complex flow features and thermal phenomena such as fuel-air mixture preparation, turbulence distribution and charge motion takes place, which are vital elements of spark ignition engine simulations. For successful and predictive simulation of engines, complete fuel & combustion chemistry, complex flow features of turbulent flow, gas exchange phenomena and combustion models are required to validate the model.

Simeon Iliev et al [8] numerically investigated alcohol blends with gasoline. This study was carried out using AVL boost and ethanol and methanol blends were compared with base gasoline. With same operating conditions, ethanol addition results in decrease of engine brake power for both high and low speed conditions. Small addition of methanol (M5 and M10) engine brake power increases. Blending of both methanol and ethanol results in reduction of CO and HC emissions. Michele Battistomi et al [9] conducted Numerical simulations using CONVERGE CFD. Experimental results were used to validate the numerical model. Results showed that in-cylinder combustion behaviour can be predicted using turbulence, combustion models and detailed chemistry.

In the reported study, Experimental analysis is conducted for base gasoline and blends of M10 & M20 (10% and 20% of methanol by volume). These experimental results are used as reference to calibrate and validate numerical model. Equations for conservation of mass, momentum and energy are solved transiently in one dimensional (along main flow direction in engine pipes) using AVL Boost CFD code [8]. System boundaries and engine pipes were initialized to atmospheric conditions and proper valve events were assigned. With the calibrated model detailed validation study was conducted.

2. Experimental Setup
The experimental set-up is shown in Fig.1. It is an 800cc 3-cylinder engine which has two valve per head. It features PFI (Port Fuel Injection). Specifications of the engine are mentioned in the below, Table 2.1. Rated power of engine dyno was 160 kW. CCS controls the thermal system and maintains inlet coolant temperature within the tolerance of 2 °C. Blend of Ethylene glycol (30%) and Water (70%) was used as coolant. Five gas analyser of make Horiba (Model: Mexa 584L) was used to take readings before and after catalytic converter.

![Fig. 2.1 Schematic Diagram of Experimental Setup](image_url)

**Fig. 2.1 Schematic Diagram of Experimental Setup**
(1) Base (2) Engine (3) Dyno (4) Engine Controller (5) Fuel Tank (6) Coolant Conditioning System (CCS) (7) Five Gas Analyser (8) Data Logging System (9) Water Tank
3. Computational Methodology

To investigate the effect of methanol-gasoline blends in PFI IC engines a schematic diagram is sketched in 1-D simulation tool AVL Boost. Numerical model was created and was validated using the experimental data as reference. Validated numerical model was used to simulate the performance characteristics of various blend compositions. This data has been validated using experimental results. To predict combustion phase duration with blended fuel correlations available for laminar burning velocity of methanol-gasoline blends are used.

System level simulation is performed using the software AVL BOOST, to study the performance of an engine operating on blends of methanol and gasoline. Primary step in 1-D modelling involves, creation of schematic sketch (which resemble functions of experimental setup) using elements available in AVL toolbox.

Table 2.1 Engine specifications

| Data                | Value          |
|---------------------|----------------|
| Number of Cylinders | 3              |
| Cycle               | 4 stroke       |
| Bore                | 68.5 mm        |
| Stroke              | 72 mm          |
| Connecting rod length | 160 mm  |
| Compression ratio   | 8.8            |

Representations used in Fig 3.1 are as follows E1 for engine while C1, C2 and C3 represents three cylinders of the engine. MP1 to MP7 are measuring probes (whose locations can be specified internally). PL stands for plenum and SB for system boundary. Numbers 1 to 26 represents pipe connectors and R1 to R6 stands for restrictions. CAT1 represents catalyst and I1 to I3 represents injectors.
System boundaries and engine pipes were initialized to atmospheric conditions and proper valve events were assigned. Prediction of combustion rates and combustion phase duration was simulated using correlations, available for laminar burning velocity of methanol-gasoline blends.

For 1-D simulation additional to engine parameters valve events are important. For the selected engine valve events are tabulated in Table 3.2

| Valve Event            | Crank angle (deg) |
|------------------------|-------------------|
| Intake Valve Open (IVO)| 55 BTDC           |
| Intake Valve Close (IVC)| 25 ATDC           |
| Exhaust Valve Open (EVO)| 80 BTDC           |
| Exhaust Valve Close(EVC)| 85 ATDC           |

To predict the combustion within the cylinder Vibe two zone model is utilized. As in the nomenclature it splits the computational domain into burned and unburned gas domains. Temperature difference is assigned to fresh charge and burned charge through the first law of thermodynamics [8].

Vibe two zone model,

\[
\frac{dm_{ub}}{da} = -P_e \frac{dv_b}{da} + \frac{dQ_e}{da} - \sum \frac{dQ_{wb}}{da} + h_w \frac{dm_b}{da} + h_{BB,u} \frac{dm_{BB,u}}{da}
\]

(1)

\[
\frac{dm_{ub}}{da} = -P_e \frac{dv_u}{da} - \sum \frac{dQ_{ub}}{da} + h_w \frac{dm_b}{da} + h_{BB,u} \frac{dm_{BB,u}}{da}
\]

(2)

Where, \(dm_u\) represents the change in the internal energy of the system, \(P_e \frac{dv_u}{da}\) is the work done by piston, \(dQ_e\) fuel heat input, \(dQ_{wb}\) is heat loss from Wall, \(h_w \frac{dm_b}{da}\) is the flow of enthalpy from the unburned to burned zone by combustion of fuel mass, \(h_{BB,u} \frac{dm_{BB,u}}{da}\) is the enthalpy due to Blow by, and subscripts b, u stands for burned and unburned gases respectively.

In addition, sum of volume zones of burned (\(V_b\)) and unburned gases (\(V_u\)) must be equal to cylinder volume (\(V\)).

\[V_b + V_u = V\]

(3)

\[\frac{dv_b}{da} + \frac{dv_u}{da} = \frac{dv}{da}\]

(4)

The rate of combustion and mixture burned is predicted using Vibe function transiently.

4. Results and Discussion

Created numerical model is calibrated and validated using the experimental results. Using the validated numerical model case studies were performed.

4.1. Calibration of the numerical model

The present study focuses on the performance characteristics of the methanol-gasoline blends. Experimental investigations were performed using base gasoline and the concentrations of 10% and 20% for part load conditions and in the speed range of 1000 to 5000 rpm. Numerical models such as combustion model, flow parameters and friction values were calibrated using recorded results for
gasoline 2500 rpm under full load conditions as reference. The variations in results were insignificant after 15 cycles but to ensure convergence 30 cycles were simulated.

| Parameter | Experimental | Simulation | Error (%) |
|-----------|--------------|------------|-----------|
| Power (kw) | 13.68        | 13.4       | 2.05      |
| Torque (Nm) | 52.28      | 51.25      | 1.97      |
| BSFC (g/kW.h) | 336.76    | 321        | 4.46      |

Combustion vibe model parameters and frictional load on engine was modified. With the above modifications numerical model was able to predict the performance characteristics with the tolerance tabulated in Table 4.1.

4.2. Validation of the numerical model
Created numerical model was subjected to parametric investigations of varying speed conditions also for methanol-gasoline blends. Base gasoline, Methanol 10% and 20% by volume (M10 & M20 respectively) were tested for speed ranges of 1000 rpm, 2500 rpm and 5000 rpm.

![Engine Power Vs Speed](image1)

Fig 4.1: Validation for Engine power

![Engine Torque Vs Speed](image2)
To simulate the performance characteristics accurately, gas exchange phenomena, combustion models and fuel chemistry are to be modelled as close to experimental behaviours. From the results it is observed that, simulation of different methanol composition resulted changes in performance characteristics. This was well captured in the in-built fuel chemistry available in AVL Boost. All the simulation results were compared with experimental results and the maximum deviation in power, torque and BSFC were within 5%.

4.3 Case Studies
Using the validated model more case studies were conducted to investigate effect of methanol addition in PFI Spark ignition IC engines. Investigations on performance characteristics were performed for base gasoline case, M10, M20, M30, M40 and M50. Engine power, Torque and BSFC characteristics for the speed ranges of 1000 rpm, 2500 rpm, 3500 rpm, 4000 rpm and 5000 rpm at full throttle conditions are simulated and plotted below.

In the speed range of 1000 rpm to 4000 rpm, with M10 as fuel engine power id not vary significantly when compared with base gasoline, but at higher speed ranges (above 4000 rpm) engine power
decreased for M10, M20 and M30. For M20, M30, M40 and M50 a steady increase in engine power was observed in the speed range of 1000 rpm to 4000 rpm. Engine power signifies the rate of work done. Methanol addition resulted in reduced combustion phase time. At higher rpms (above 4000 rpm) more amount of work has to be done on piston, more fuel is to be burned and more heat has to be released, because of low calorific value of methanol (20 MJ/kg) heat generated reduces. This proportionately reduces the work done.

![Engine Torque Vs Speed](image)

**Fig 4.5** Engine torque variation with methanol blends

Engine torque corresponds to the ability to perform work. With methanol addition of 10% by volume engine torque exhibited similar trend as that of gasoline in all the speed ranges except 3500 rpm. Remaining all the blends for all the speed ranges, torque produced by blended fuel higher than base gasoline in the speed range of 1000 rpm to 5000 rpm. In the speed range of 1000 rpm to 3500 rpm M20 and M50 produced highest torque. But at higher speeds (above 4000 rpm) M20 had similar torque values as that of base gasoline. M50 produced higher torque compared to baseline case for all the speed ranges. With M50 as fuel, the improvement in torque at 2500 rpm was 6.8 % and at 3500 rpm 1.76 %.

![BSFC Vs Speed](image)

**Fig 4.6** BSFC variation with methanol blends
From the results, it was observed that BSFC characteristics significantly varied with methanol composition. With increase in methanol composition BSFC increased in the speed range of 1000 rpm to 5000 rpm compared to base gasoline except for M10 during 1000 rpm to 3500 rpm. From the results, it was observed that at lower speeds, BSFC increases significantly for blended fuel. But at higher rpms improves thermal efficiency. In the Fig 4.6, at 1000 rpm M40 has 24% higher BSFC but at 5000 rpm this difference is only 2%. Close to maximum rated speed (5000 rpm) methanol blends of M10, M20 and M30 showed lower BSFC readings compared to baseline case. This is because of the high volatile nature of methanol, which supports shorter combustion duration. But when methanol composition increased to M40 and M50 due to lower calorific value of methanol BSFC increased. Remaining all speed conditions BSFC increased proportionately with methanol composition. Maximum increase in BSFC for M50 was observed at 4000 rpm was 25.7% compared to base gasoline.

5. Conclusions
Numerical model was created and calibrated and validated A significant change in engine performance characteristics is exhibited with change in methanol composition over speed range of 1000 rpm to 5000 rpm. From the performance characteristics, M10 & M20 showed better compatibility to the engine compared to other fuel blends. With M20, Power and Torque was improved for the speed range of 1000 rpm to 4000 rpm. At maximum rated speed (5000 rpm) engine power and torque showed a reduction of 3.9% and 2.5% respectively. Compared to base gasoline, BSFC of M20 was higher than base gasoline case in the speed range of 1000 rpm to 2500 rpm (low speeds) and at higher speeds (2500 rpm to 5000 rpm), BSFC reduced compared to baseline case. Influence of blends was significant at higher speeds.

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