COMPUTATIONAL AND EXPERIMENTAL STUDY OF ENGINE CHARACTERISTICS USING N-BUTANOL GASOLINE BLENDS

S Raviteja¹, Shashank S N¹ and Kumar G N²

¹ Student, Department of Mechanical Engineering, National Institute of Technology Karnataka Surathkal, Mangalore, India- 575025
² Assistant Professor, Department of Mechanical Engineering, National Institute of Technology Karnataka Surathkal, Mangalore, India- 575025

ABSTRACT

This study investigates the effect of blending of n-butanol with gasoline in a four-stroke spark ignited MPI engine. AVL BOOST was used as a computational fluid dynamics (CFD) simulation tool to analyze the performance and emission characteristics for different blends of n-butanol and gasoline (0%, 10%, 20% and 30% of butanol by volume). The study was carried out at full load conditions for different engine speeds. CFD results are always approximate due to truncation errors. An experiment was conducted on a four-cylinder spark ignited MPI engine to validate the results obtained from AVL Boost. AVL simulation and experimental results showed a considerable decrease in Hydro-Carbon (HC) Emissions and the percentage of Carbon Monoxide (CO) emitted remained constant. However, an increase in emissions of Oxides of Nitrogen (NOx) was observed in both cases.

Keywords: AVL Boost, CFD, Emissions, n-Butanol blends, Variable speed

1. INTRODUCTION

The Dwindling crude oil reserves and the long lead times in creating these fuels have brought in the fear of fuel crisis in the near future. The known worldwide reserves of petroleum are about 1000 billion barrels and these petroleum reserves are predicted to be consumed in about 30 years. Increasing Air pollution is one of the other major problems being faced by the world today. This has led to a debate on usage of alternate fuels which have the potential to replace gasoline. Alcohols are advocated as the prospective fuels because they can be manufactured from natural products or waste materials, unlike gasoline which is a non renewable energy resource. Alcohols can be used directly without requiring
any major changes in the structure of the engine. Ethanol was the first fuel among the alcohols used to power vehicles in the 1880s and 1890s [1]. However, economic reasons still limit its usage on a large-scale.

Butanol has a 4-carbon structure with a hydroxyl group (-OH) attached to one of the carbon atoms. There exist different isomers of butanol based on their molecular structure. n-Butanol has a straight chain structure. Various properties of n-Butanol in comparison with fossil fuels and few other alcohols have been presented in the TABLE 1. Studies have shown that n-butanol is more advantageous over the lighter alcohols like ethanol and methanol. n-Butanol has higher energy content when compared to ethanol, which reduces the Specific Fuel Consumption. n-Butanol is also less prone to water contamination and is less volatile in comparison to ethanol. As a result it could be distributed and stored using the same infrastructure used for gasoline. n-Butanol has a higher heat of evaporation. n-Butanol has lower volatility, which reduces the tendency of cavitation and vapour lock. n-Butanol has a lesser heat of vaporization, which enables easy cold start. n-Butanol has a very low vapour pressure and high flash point, which makes it a safe fuel [2].

n-Butanol can be produced from both petrochemicals as well as from renewable resources like agricultural waste. Historically, n-Butanol was produced by biological fermentation processes. The advent of biotechnology has made possible many new advanced chemical and biological ways of butanol production [3]. Butanol production from fermentation process of agricultural feedstock by cellulosic enzymes has the potential to cut its production cost [4]. However the studies investigating the use of Butanol in internal combustion engines are very limited. This study investigates the effect of n-Butanol gasoline blends in a Spark Ignited Internal Combustion Engine.

Table 1: Property of different fuels

<table>
<thead>
<tr>
<th></th>
<th>Gasoline</th>
<th>Methanol</th>
<th>Ethanol</th>
<th>n-Butanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular formula</td>
<td>C₄-C₁₂</td>
<td>CH₃OH</td>
<td>C₂H₅OH</td>
<td>C₄H₉OH</td>
</tr>
<tr>
<td>Octane Number</td>
<td>80-99</td>
<td>111</td>
<td>108</td>
<td>96</td>
</tr>
<tr>
<td>Oxygen content(%)</td>
<td></td>
<td>50</td>
<td>34.8</td>
<td>21.6</td>
</tr>
<tr>
<td>Density(g/mL) at 20˚C</td>
<td>0.72-0.78</td>
<td>0.796</td>
<td>0.790</td>
<td>0.808</td>
</tr>
<tr>
<td>Auto-ignition</td>
<td>300</td>
<td>470</td>
<td>434</td>
<td>385</td>
</tr>
<tr>
<td>Temperature(˚C)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lower Heating</td>
<td>42.7</td>
<td>19.9</td>
<td>26.8</td>
<td>33.1</td>
</tr>
<tr>
<td>Value(MJ/kg)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Latent Heating (kJ/kg) at 25˚C</td>
<td>380-500</td>
<td>1109</td>
<td>904</td>
<td>582</td>
</tr>
<tr>
<td>Stoichiometric ratio</td>
<td>14.7</td>
<td>31.69</td>
<td>13.8</td>
<td>2.27</td>
</tr>
<tr>
<td>Boiling Point(˚C)</td>
<td>25-215</td>
<td>64.5</td>
<td>78.4</td>
<td>117.7</td>
</tr>
</tbody>
</table>

The advent of high-speed digital computers and advances in Computational methods has made it possible for the researchers to simulate and analyse complex physiological processes. The huge amount of results that are obtained by simulation studies are rather very difficult to be obtained experimentally. The use of Computational Fluid Dynamics (CFD) further saves upon the manpower, material and financial resources. CFD has been looked
upon as a high-technology research and design tool by the automobile researchers. The ability to analyse not only the external flows but also the flows in the manifolds and engine cylinders has made the use of CFD essential before actual experimentation. Advances in Computational algorithms have helped researchers to even simulate the combustion process happening within the cylinder [5]. The present study uses CFD to simulate the combustion process of butanol blends in IC Engine.

2.  BACKGROUND

Investigation of butanol usage as an engine fuel has been conducted by several research groups. Alasfour reported that there was an increase in first and second-law efficiencies in the lean regions for the butanol-gasoline blend; also investigations were made on the effect of spark timing on the NO\textsubscript{x} production for a engine running on 30% iso-butanol-gasoline engine [6, 7]. J. Dernotte et al assessed influence of butanol addition on the emission of unburned hydrocarbons, carbon monoxide, and nitrogen oxide using different butanol–gasoline blends in a port fuel-injection, spark-ignition engine. The studies reported that 40% butanol/60% gasoline blend by volume (B40) minimized HC emissions, no significant change in NO\textsubscript{x} emissions except B80, which showed lower emission levels due to combustion deterioration [8]. Studies by S. Szwaia and J.D. Naber reported that Combustion stability at the part-load condition as measured by the COV of IMEP was slightly lower for n-butanol in comparison to gasoline using blends of n-butanol to gasoline with ratios of 0%, 20%, and 60% in a single cylinder Waukesha Cooperative Fuels Research engine (CFR) SI engine with variable compression ratio [4]. Xiaolei Gu et al analysed the effect of spark timing, blend ratio and EGR rate on the emission characteristics. Results showed that the blends of gasoline and n-butanol decrease engine specific HC, CO and NO\textsubscript{x} emissions compared to those of gasoline. It was also examined that EGR reduces engine specific NO\textsubscript{x} emissions and particle number concentration simultaneously in spark-ignition engine fuelled with gasoline and n-butanol blends [9]. Experimental tests were carried out by G. Broustail et al on a single-cylinder port-fuel injection SI engine to quantify the potential of butanol/iso-octane blends to reduce regulated pollutants (CO, CO\textsubscript{2}, NO\textsubscript{x} and HC), and non-regulated pollutants (methane, acetylene, ethylene, benzene, acetaldehyde and formaldehyde), without deteriorating the engine performance. It was reported that there was an increase of the fuel consumption of about 30% with butanol and 60% with ethanol, but only a slight increase (about 2%) in CO\textsubscript{2} emissions. A strong decrease in HC and NO\textsubscript{x} emissions was obtained for both alcohols [10]. Adrian Irimescu investigated the effect of fuelling a port injection engine with iso-butanol, as compared to gasoline operation. Fuel conversion efficiency decreased when the engine was fueled with iso-butanol by up to 9% at full load and by up to 11% at part load. He cited incomplete fuel evaporation as the reason for the drop in engine efficiency [11]. In his additional investigations, it was found that Iso-butanol can be blended with gasoline in much higher concentrations compared to ethanol, without any modifications to the fuel system or other engine components [12].

3.  PRESENT WORK

AVL Boost is a package of computer codes which enables the user to model and simulate the various processes of an Internal Combustion Engine. In the current investigation AVL BOOST has been used to analyze effect the blending of n-Butanol (C\textsubscript{4}H\textsubscript{10}O) with
gasoline at different concentrations. Blends of n-Butanol to gasoline with ratios of 0%, 10%, 20%, and 30% by volume were used in the simulation for various speed conditions. Due to the fact that CFD results are always approximate, Engine Test bed experiments were conducted to validate the results obtained from the simulations. One of the purposes of this paper is to analyze the computed results and their deviation from the experimental results.

4. SIMULATION MODELLING

The pre-processing steps of AVL Boost enables the user to model a 1-Dimensional engine test bench setup using the predefined elements provided in the software toolbox. The various elements are joined by the desired connectors to establish the complete engine model using pipelines.

In Fig.1, E1 represents the engine C1, C2, C3, C4 represent the four cylinders of the engine. MP1 to MP14 represent the measuring points, PL1, PL2 represent the plenum. SB1, SB2 are for the system boundary and the flow pipes are numbered 1 to 32. CL1 represents the cleaner and R1 to R10 represent flow restrictions.

Figure 1: AVL BOOST 1D Engine model

The various configurations and parameters are set for each element. The system boundary conditions are specified. It is important to make a correct estimate of the boundary conditions as it directly affects the accuracy of the results.

For the current study Vibe two zone model was selected for the combustion analysis. This model divides the combustion chamber into unburned and burned gas regions [13]. The first law of thermodynamics is applied to each of the zones to predict the rate of fuel consumed with respect to crank angle.
The following equations (1, 2) govern the Vibe two zone model [14]:

\[
\frac{dm_u}{da} = -p_c \frac{dV_b}{da} + \frac{dV_f}{da} - \sum \frac{dQ_{WB}}{da} + h_u \frac{dm_b}{da} - h_{BB,b} \frac{dm_{BB,b}}{da}
\]  

(1)

\[
\frac{dm_u}{da} = -p_c \frac{dV_u}{da} - \sum \frac{dQ_{WB}}{da} - h_u \frac{dm_b}{da} - h_{BB,u} \frac{dm_{BB,u}}{da}
\]  

(2)

Where

\(dm_u\) Denotes change of the internal energy in the cylinder

\(p_c \frac{dV_c}{da}\) Denotes piston work

\(\frac{dQ_f}{da}\) Denotes fuel heat input

\(\frac{dQ_{WC}}{da}\) Denotes wall heat losses

\(h_u \frac{dm_c}{da}\) Denotes enthalpy flow from the unburned to the burned zone

\(h_{BB,c} \frac{dm_{BB,c}}{da}\) Denotes enthalpy due to blow by

\(u\) and \(b\) in the subscripts denote unburned and burned gas

Prediction of NOx generated by combustion was based on the model by Pattas and Häfner which incorporates the well known Zeldovich mechanism [15]. The rate of NOx production was estimated by using the following equation (3):

\[
r_{NO} = C_{PPM} \cdot C_{KM} \cdot (2.0) \cdot (1 - a^2) \cdot \frac{r_1}{1 + \alpha AK_2} \cdot \frac{r_4}{1 + AK_4} 
\]  

(3)

\[
\alpha = \frac{c_{NO,act}}{c_{NO,equ}} \cdot \frac{1}{C_{PPM}}
\]

\[
AK_2 = \frac{r_1}{r_2 + r_3} \quad AK_4 = \frac{r_4}{r_5 + r_6}
\]

Where

\(C_{PPM}\) Denotes Post Processing Multiplier

\(C_{KM}\) Denotes Kinetic Multiplier

\(c\) Denotes molar concentration in equilibrium

\(r_i\) Denotes reactions rates of Zeldovich mechanism
The amount of CO emissions was predicted using the following equation (4) which was taken from a model presented by Onorati et al[16].

\[ r_{CO} = C_{\text{const}} \cdot (1 - \alpha) \cdot (r_1 + r_2) \]  

\[ \alpha = \frac{c_{\text{CO,act}}}{c_{\text{CO,equ}}} \]

Where
- \( c \) Denotes molar concentration in equilibrium
- \( r \) \(_1\) Denotes reactions rates based on the model

The process of formation of unburned hydrocarbons in the crevices is described by assuming that, the pressure in the cylinder and in the crevices is the same and that the temperature of the mass in the crevice volumes is equal to the piston temperature [17].

The mass in the crevices at any time period is given by equation (5):

\[ m_{\text{crevice}} = \frac{p \cdot V_{\text{crevice}} \cdot M}{R \cdot T_{\text{piston}}} \]  

Where
- \( m_{\text{crevice}} \) Denotes mass of unburned charge in the crevices [kg]
- \( p \) Denotes cylinder pressure [Pa]
- \( V_{\text{crevice}} \) Denotes total crevice volume [m3]
- \( M \) Denotes unburned molecular weight [kg/kmol]
- \( R \) Denotes gas constant [J/(kmol K)]
- \( T_{\text{piston}} \) Denotes piston temperature [K]

Butanol properties are not pre-defined in AVL BOOST. Hence coefficients for calculating thermodynamic properties of Butanol were taken from NASA Technical Memorandum [18] and were added to the BOOST fuel database to simulate the engine fuelled with the blends.

5. EXPERIMENTAL SETUP AND EXPERIMENTS

The engine setup consists of a four-stroke, four cylinder, SI engine as shown in the Fig. 2. The setup had stand-alone panel box consisting of air box, fuel tank, manometer, fuel measuring unit, transmitters for air and fuel flow measurements, process indicator and engine indicator. Rotameters were provided for cooling water and calorimeter water flow measurement. The setup enables study of engine performance for brake power, indicated power, frictional power, BMEP, IMEP, brake thermal efficiency, indicated thermal efficiency, mechanical efficiency, volumetric efficiency, specific fuel consumption, air-fuel ratio (A/F) and heat balance. Windows based engine performance analysis software package ‘Engine Soft’ is provided for on-line performance evaluation.
AVL 5 gas exhaust analyser was used to obtain the emission characteristics. TABLE 2 gives the range and resolution of the analyser. TABLE 3 gives the technical specifications of the engine used for the experiments.

### Table 2: Range and Resolution of the AVL exhaust gas analyser

<table>
<thead>
<tr>
<th>Measured Parameters</th>
<th>Measured Range</th>
<th>Resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>0-10% Vol.</td>
<td>0.01% Vol.</td>
</tr>
<tr>
<td>HC</td>
<td>0-20000 ppm</td>
<td>10 ppm</td>
</tr>
<tr>
<td>CO₂</td>
<td>0-20% Vol.</td>
<td>0.1% Vol.</td>
</tr>
<tr>
<td>O₂</td>
<td>0-22% Vol.</td>
<td>0.01% Vol.</td>
</tr>
<tr>
<td>NO</td>
<td>0-5000 ppm</td>
<td>1 ppm</td>
</tr>
</tbody>
</table>

### Table 3: Specifications of the Engine

<table>
<thead>
<tr>
<th>Make</th>
<th>Suzuki</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>Zen MPFI</td>
</tr>
<tr>
<td>Type</td>
<td>4 Cylinder, 4 stroke</td>
</tr>
<tr>
<td>Capacity</td>
<td>993 cc</td>
</tr>
<tr>
<td>Cooling</td>
<td>Water Cooled</td>
</tr>
<tr>
<td>Max. Power</td>
<td>44.5kW @ 6000rpm</td>
</tr>
<tr>
<td>Max. Torque</td>
<td>59Nm @ 2500rpm</td>
</tr>
<tr>
<td>Stroke</td>
<td>61mm</td>
</tr>
<tr>
<td>Bore</td>
<td>72mm</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>9.4:1</td>
</tr>
</tbody>
</table>
6. RESULTS AND DISCUSSION

The present study concentrated on the emission and performance characteristics of the n-butanol-gasoline blends. Different concentrations of the blends (10% n-Butanol (B10), 20% n-Butanol (B20) and 30% n-Butanol (B30) by volume) were analysed using AVL BOOST codes and were validated experimentally at full load conditions for the speeds ranging from 2000-4000 rpm in the steps of 500rpm. The results are divided into different subsections based on the parameter analysed.

6.1 Brake Power

Brake power is one of the important factors that determine the performance of an engine. The variation of brake power with Speed was obtained at full load conditions for B10, B20, B30 and pure gasoline using the CFD results. The results were also validated experimentally and it was found that there was a very small deviation in CFD results from the experimental results. This can be clearly seen in Fig. 3 to Fig. 6.

Figure 3: Variation of Brake Power with speed for pure Gasoline

Figure 4: Variation of Brake Power with speed for case of B10

Figure 5: Variation of Brake Power with speed for B20

Figure 6: Variation of Brake Power with speed for B30
The deviation noted in all the four cases is very small and occurs due to the assumptions made during the CFD analysis as well as the human errors made during the experiments. The results show that the brake power increases in the cases of B10 and B20 compared to Pure Gasoline. However there was a decrease in case of B30. This factor can be acknowledged to the lower heating value of n-Butanol compared to Gasoline.

6.2 CO Emissions

Carbon Monoxide (CO) emission is a strong function of equivalence ratio. The influence of other parameters on the emissions of CO is very low and the percentage of CO emitted from the engine was almost constant with increasing speed at full load condition. The variation of CO emissions with respect to speed for different blends is shown below in Fig. 7 to Fig.10.

Both CFD and experimental results show that the change in percentage of CO emissions with varying speed is constant at full load conditions for all the cases.
The emission of CO increases for B10 and drastically decreases for B20 and B30. This decrease can be attributed for the presence of extra oxygen molecule in n-Butanol which helps in more complete combustion and thus decrease in amount of CO.

6.3 NO\textsubscript{x} Emissions

NO\textsubscript{x} emissions are mainly affected by the equivalence ratio, peak temperature, ignition timing and oxygen concentration in the fuel. In the present study, NO\textsubscript{x} emissions were obtained from CFD analysis and the results were validated experimentally. Both the results have shown that there was increase in NO\textsubscript{x} emissions with increase in speed. B10, B20, B30 showed an increase in NO\textsubscript{x} emissions because of the increase in oxygen concentration. The CFD and Experimental results are shown for various cases in Fig. 11 to Fig.14.
6.4 HC Emissions

The origin of unburned hydrocarbons (HC) in SI Engines is due to incomplete combustion of charge. Major source of HC emission is the charge in the crevice volume which is not burned due to flame quenching at the entrance and fuel vapours absorbed by the oil layers are not burned during the combustion process. Variations of HC emitted with respect to speed are shown Fig.15 to Fig.18.

From the results obtained, it is clear that HC emissions decrease with increase in percentage of n-butanol. However experimentally obtained results showed a considerable deviation from CFD results. This is due to the fact that a complete description of the HC formation process cannot yet be simulated and the achievement of a reliable predictive model within a thermodynamic approach is prevented by the fundamental assumptions and the requirement of reduced computational times [14]. AVL BOOST code predicts the formation of HC based on G. D'Errico model. n-Butanol is not readily available in the AVL database and considers
only thermodynamic and transport properties for the prediction of combustion. However fuel specific properties are not considered. Laminar flame speeds of alcohols are higher compared to gasoline. Hence this leads to better combustion at higher engine speeds and decrease in HC emissions which are not accounted by the software.

7. CONCLUSIONS

CFD and experimental analysis was carried out successfully on SI Engine and the following conclusions are made based on the results.

- CFD and experimental results complement each other for the performance characteristics at full load conditions for all blends.
- CO emissions remained constant experimentally for all blends as predicted by the CFD simulations.
- NO emissions were estimated to increase with the increase in butanol concentration by AVL BOOST and were successfully validated by the experiments.
- CFD results showed a considerable deviation in forecasting HC emissions when compared to the experiments.

8. ACKNOWLEDGEMENTS

The authors would like to acknowledge AVL-AST, Graz, Austria for granted use of AVL-BOOST under the university partnership program. We are also eternally grateful to staff members of NITK Surathkal for their immense support.

REFERENCES