

Butanol-Diesel Blends for Partially Premixed Combustion

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ABSTRACT

Partially Premixed Combustion has shown the potential of high efficiency, emissions of nitrogen oxides (NO_x) and soot below future emissions regulations, and acceptable acoustic noise. Low-octane-number gasoline fuels were shown to be most suitable for this concept, with the reactivity determining the possible load range. Other researchers have used several refinery streams, which might be produced by a refinery if they were required to do so without additional investment.

Some of refinery streams are, however, not expected to be commercially available on the short term. For the present investigation, *n*-butanol (BuOH) has been selected as a blend component in diesel, and is used from 50 - 100%. The blends then have a reactivity range similar to the refinery streams, so single-cylinder engine tests for their emission and efficiency performance can also be used to determine their applicable load range.

The current paper presents a summary of the performance of such BuOH-diesel blends with respect to emissions and efficiency in the Partially Premixed Combustion regime. Besides a presentation of the sensitivity to injection strategies, dilution levels and fuel pressure, emission performance is compared to upcoming legislated emission levels. The effect of the blend ratio on load ranges is shown and conventional diesel combustion benchmarks are used to show improvements in indicated efficiency.

Butanol-diesel blends are shown to be a viable approach to partially premixed combustion, with its high soot reduction potential and stable operation. EURO VI emission levels can therefore be achieved, with moderate or slightly increased fuel pressure. Combustion efficiency is shown to be very reasonable over the whole load range, similar to that of conventional diesel combustion. Combined with an improved thermal efficiency a moderate butanol-diesel blend is shown to have an average gross indicated efficiency of 50% over the whole load range.

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INTRODUCTION

Diesel engines are known for their relatively high efficiency, but traditionally suffer from significant emission levels of both particulate matter (PM) and nitrogen oxides (NO_x) [1]. Over the past decades, manufacturers have largely overcome these harmful emissions by introducing new technologies, e.g. high pressure fuel injection equipment [2] and advanced exhaust gas after treatment [3]. These have not only added significant extra costs to vehicles, but have also broken the trend of ever increasing engine efficiency [4].

Partially Premixed Combustion [5, 6, 7] has shown the potential of further increasing engines' efficiency, with emissions of NO_x and soot below future emissions regulations, and acceptable acoustic noise. With conventional fuels, i.e. diesel [8] or gasoline [9], several challenges exist, but relatively low-octane-number gasoline fuels [10] were shown to be very well suitable for this concept. The reactivity

of the fuels was shown to be determining the possible load range, which at best ranges from idle to full load, without major modifications to the engine setup. Both the groups of Saudi Aramco [10] and Lund [11] have used refinery streams, upstream precursors of conventional gasoline.

Such refinery streams are, however, not expected to be commercially available on the short term. For certain applications, the use of conventional diesel blended with a promising second-generation biofuel of low-reactivity and relatively high-volatility could provide a viable approach. That is, if such a blend can give similar emission advantages as the earlier mentioned refinery streams, and has a suitable load range.

Furthermore, the bio-component could provide additional advantages, such as the soot-reducing effects of atomic oxygen and a further reduction in effective carbon dioxide emissions. For the present investigation, *n*-butanol (BuOH) has been selected as a blend component.

Butanol is thought to be an important future fuel component [12]. It has excellent properties for blending with gasoline (especially branched or *t*-butanol) [13]. Nevertheless, the more reactive isomer, *n*-butanol, could be suitable for PPC purposes. The high oxygen content of 21 wt-% is likely to contribute to low soot emissions and its relatively high heat of vaporization (~ 52.3 kJ/mole) is beneficial for lowering in-cylinder temperatures [14].

Moreover, butanol is of particular interest since it can be derived from biomass [15], like ethanol. Furthermore, butanol is favorable over ethanol for several reasons. It has a higher energy density, is less hygroscopic than ethanol¹ and is less corrosive to several metals and polymers. Existing infrastructure could thus be used for transportation. Moreover, the lubricity is sufficiently high.

Nevertheless, pure bio-butanol or high butanol content blends in a diesel engine have not been investigated yet. Bio-butanol can be directly used as gasoline fuel and the possibility to blend it with diesel in significant amounts (up to 40%) was shown in a recent publication by Istituto Motori [17].

In the present paper butanol fractions of 50 to 100% are used. The blends then have a reactivity range similar to the refinery streams which were mentioned before, so single-cylinder engine tests for their emission and efficiency performance can also be used to determine their applicable load range.

The current paper presents a summary of the performance of the BuOH-diesel blends with respect to emissions and efficiency in the Partially Premixed Combustion regime. Besides a presentation of the sensitivity to injection strategies, dilution levels and fuel pressure, emission performance is compared to upcoming legislated emission levels. The effect of the blending ratio on load ranges is shown and conventional diesel combustion benchmarks are used to show improvements in indicated efficiency.

EXPERIMENTAL SETUP

Experimental Apparatus

For this investigation a six-cylinder DAF engine, referred to as CYCLOPS, is used. For more information on the setup the reader is referred to a detailed description [8], of which this subsection is a short summary. Prior to this measurement campaign, the engine has been overhauled with new pistons and liners.

The CYCLOPS is a dedicated engine test rig, see Table 1, based on a DAF XE 355 C engine. The pistons are of a low-compression XE390c version, which together with the thickest head gasket available (1.45 mm) yield a compression ratio of 15.7. Cylinders 4 through 6 of this inline 6 cylinder HDDI engine operate under the stock DAF engine control unit and together with an eddy-current dynamometer they are

only used to control the crankshaft rotational speed of the test cylinder, i.e. cylinder 1. Apart from the mutual cam- and crankshaft and the lubrication and coolant circuits, this test cylinder operates autonomously from the propelling cylinders and uses stand-alone air, EGR and fuel circuits for maximum flexibility.

Table 1. CYCLOPS test setup specifications

Base Engine	6 cylinder HDDI diesel
Cylinders	1 Test cylinder
Bore [mm]	130
Stroke [mm]	158
Compression ratio	15.7 (original 17.0)

Fed by an air compressor, the intake air pressure of the test cylinder can be boosted up to 5 bar. Non-firing cylinders 2 and 3 function as EGR pump cylinders (see Figure 1), the purpose of which is to generate adequate EGR flow, even at 5 bar charge pressure and recirculation levels in excess of 70%. The EGR flow is cooled both up- and downstream of the pump cylinders. Several surge tanks, to dampen oscillations and to ensure adequate mixing of fresh air and EGR flows, and pressure relief valves, to guard for excessive pressure in the circuit, have been included in the design.

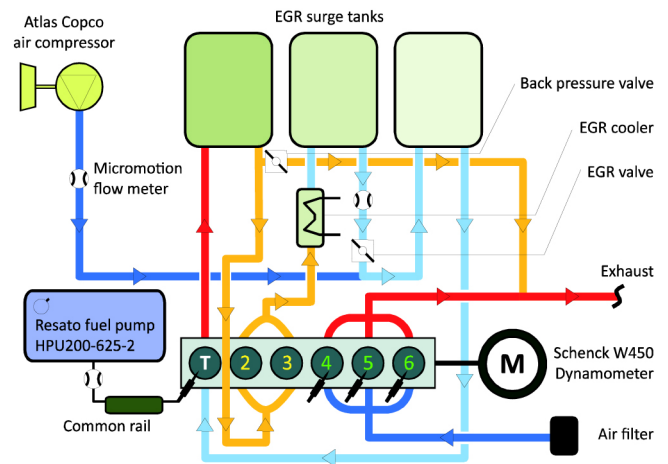


Figure 1. Schematic of CYCLOPS experimental setup: a modified DAF engine using separate fuel, air and EGR systems for one dedicated test cylinder

Direct injection of fuel into cylinder 1 is provided by a prototype Delphi common rail injector with a nozzle having 8 holes of 0.151 mm diameter with an umbrella angle of 153 degrees. All steady state flows of fuel, air and EGR are measured with Coriolis mass flow meters.

For measuring gaseous exhaust emissions, a Horiba Mexa 7100 DEGR emission measurement system is used. Exhaust smoke level (in Filter Smoke Number or FSN units) is measured using an AVL 415S smoke-meter. All quasi steady-

¹Due to its structural shape with an elongated apolar chain [16]

state engine data are recorded by means of an in house data acquisition system (TUEdACS). A SMETEC Combi crank angle resolved data acquisition system is used to record and process crank angle resolved data. For more information on the setup and the procedures and definitions used, the reader is referred to [8].

Fuel Blends Under Investigation

Table 2 gives an overview of the specifications of the fuels which are used in the blends. *N*-butanol and EN590 diesel have both been tested according to ASTM D240 (higher heating value or HHV). To obtain the lower heating value or LHV the heat released by the condensing water has been subtracted from the higher heating value.

Table 2. Fuels used for the blends

Fuel	CN	AFR	HHV [MJ/kg]	LHV [MJ/kg]	Boiling range [°C]
<i>n</i> -butanol	17 [18]	11.13	35.76	33.02	117
EN590	52.4	14.6	45.4	42.7	170-360

The *n*-butanol has been tested for any unwanted impurities in a combined gas chromatography-mass spectrometer (GC-MS), type GCMS-QP5000 from Shimadzu. Di-ethyl ether (DEE) is used as a solvent, because of its high volatility and lower boiling point compared to the test substances.

Obtained GC spectra and full compositions are presented as appendices, see Figure 20 and Table 5. As can be seen, one major peak which saturated the detector was found. Apparently, the *n*-butanol consists of almost only 1-butanol and probably some 2-butanol. Those two molecules could not be distinguished with the current settings and column. Only a minor fraction of 2-pentanol (0.13 wt-%) was found.

Five blends with relatively high butanol content (i.e. 90-80-70-60-50 vol-%) have been investigated for this research. No visual separation in the diesel-butanol blends was found over a period of a number of weeks. Apart from varying reactivity and volatility, using different blend contents also implies varying air fuel ratios and heating values due to the relatively high differences in both AFR and heating value caused by the presence of oxygen in the molecule.

The fuel blends have not been tested on a CFR engine for octane number or on an ignition quality tester for cetane number. Therefore, only a rough estimation of the reactivity of each of the blends, based on linear blending, can be given. The reference CN value for *n*-butanol, being 17, is taken from [19]. Some properties of the blends used, are given in Table 3.

Table 3. Specific parameters for the tested blends

	AFR _{st} [-]	LHV [MJ/kg]	Estimated CN [-]
BuOH90	11.48	33.99	20.5
BuOH80	11.82	34.96	24
BuOH70	12.17	35.92	27.6
BuOH60	12.52	36.89	31.1
BuOH50	12.87	37.86	34.7

Conditions and Procedure

Based on the results of Manente [20], the engine speed is set to 1250 rpm, which is typical for a heavy duty vehicle during highway cruising. An EGR flow of around 50 weight percent is used, both to limit pressure rise rates, as found in previous work [21], and nitrogen oxides emissions to levels below Euro VI [22,23].

The latter two references have stated that a combustion temperature higher than 1500K is necessary to promote the reactions from CO to CO₂, and that on the other hand it is important to be below 2000K to avoid thermal NO formation (Zeldovich' mechanism). Apart from an EGR percentage of around 50 wt-%, this also implies the use of a global lambda value of around 1.5. To achieve such an air excess ratio, intake pressure is varied accordingly.

The recirculated exhaust gas is heavily cooled using cold process water, to approximately 300K and the exhaust back pressure is regulated to 0.3 ± 0.2 bar higher than the intake pressure (to mimic the presence of a turbocharger of finite efficiency and to enable the use of external short route EGR in practice). The 0.3 bar excess exhaust pressure is considered to be feasible with sufficient high turbocharger efficiency. The error interval given is caused by test bench limitations.

Summarized, for all measurements the following conditions are kept constant:

- Engine speed = (1250 ± 10) rpm
- $\lambda = (1.5 \pm 0.1)$
- (50 ± 5) wt-% of EGR

At 8 bar gross IMEP, first the combustion behavior is tested for all blends, using a single injection strategy. After that, a double injection strategy is compared to the more conventional single injection, by varying the start of injection (SOI) until the desired CA50 is reached within ± 1 °CA.

- Single injection - five SOIs aiming at CA50s of 2, 4, 6, 8, and 10 °CA aTDC at 8 bar.
- Double injection strategy.

Furthermore, the sensitivity of combustion behavior with respect to the total dilution level will be analyzed, by increasing the intake pressure in 0.1 bar increments, keeping all other parameters constant. This results in:

- Air excess ratios ranging from 1.5 to 2.5, keeping EGR level and all other parameters constant.

Particulate emission levels from conventional diesel combustion are known to be sensitive to the fuel pressure used. Whether this is still the case when using butanol-diesel blends is tested using a fuel pressure sweep. This results in:

- Fuel pressure varying from 1400 bar down to 800 bar, with 100 bar increments.

After these sensitivity analyses, the load range of each of the fuels will be shown, for which five loads have been selected. For each target load ± 0.5 bar, the fuel mass flow is kept constant and small variations in load (originating for varying efficiencies) are allowed accordingly:

- Gross IMEPs of 8, 10, 12, 14 and 16 bar, corresponding to 32-64% of the engine's rated torque

Fuel pressure increases with load to keep injection duration roughly at a constant in crank angle domain. A moderate 1000 bar at 8 bar load is taken as starting point and with every 2 bar of load increase, fuel pressure will be increased with 200 bar.

All operating points should have acceptable combustion stability (i.e. $\sigma_{IMEP} < 5\%$) and preferably meet each of the following emission levels:

- CO emissions below 2000 ppm,
- UHC emissions below 1000 ppmC with as target below 400 ppmC,
- NO_x emissions below 200 ppm with as a target below 50 ppm to reach EURO VI,
- FSN smoke number below 1 with as a target below 0.2 to reach EURO VI.

As a consequence of the exotic operating conditions, hardware and setup limitations should be kept in mind.

- Originally, this engine has been designed for peak firing pressures of 225 bar. This limit has been lowered to 200 bar due to the highly asymmetric load on the crank shaft.
- Pressure rise rates (PRR) should not exceed a certain limit to prevent engine damage and excessive combustion noise. According to Leermakers [8], this setup has proven to work with pressure rise rates of 30 bar/°CA. Nevertheless, it is wise to lower this limit somewhat (15 bar/°CA).
- Wall wetting could lead to liner damage by means of oil dilution. As an indicator for this, the HC emissions have been limited to 2000 ppmC.

Definitions

The calculated crank angle at which 10% of the fuel has been burnt as main indicator for the start of combustion (SOC). This is used to compute relevant combustion properties such as ignition delay, ignition dwell, combustion delay and combustion duration. Moreover, the duration between end of injection and start of combustion is also defined. This so-called ignition dwell, if positive, is

beneficial for reduced soot production, i.e. injection has ended before combustion starts. These parameters can be summarized as:

- Ignition delay (ID) is defined as CA₁₀ - SOI_{main}
- Burn duration (BD) is defined as CA₉₀ - CA₁₀
- Ignition dwell is defined as CA₁₀ - EOI_{main}

Premixed fraction

It has been postulated before that Partially Premixed Combustion can vary in the amount of premixed combustion. This is quantified by comparing the heat released in the premixed combustion phase and the total heat released. The premixed fraction is defined using the method suggested by Solaka and coworkers [24] is followed, where a Gaussian profile is fitted to the rising flank of the premixed peak, between half of the maximum and the actual peak. The Gaussian profile is defined as

$$G(x) = h \cdot e^{-\frac{(x-x_0)^2}{2\alpha^2}}, \quad (1)$$

with x_0 the central position of the peak, and h and α representing the height and width of the Gaussian profile, respectively. From Figure 2 can be seen that the fit follows the premixed heat release closely. The Gaussian profile is merely a mathematical representation of the premixed reaction phase. However, it shows a robust measure of the premixed fraction for all operated cases.

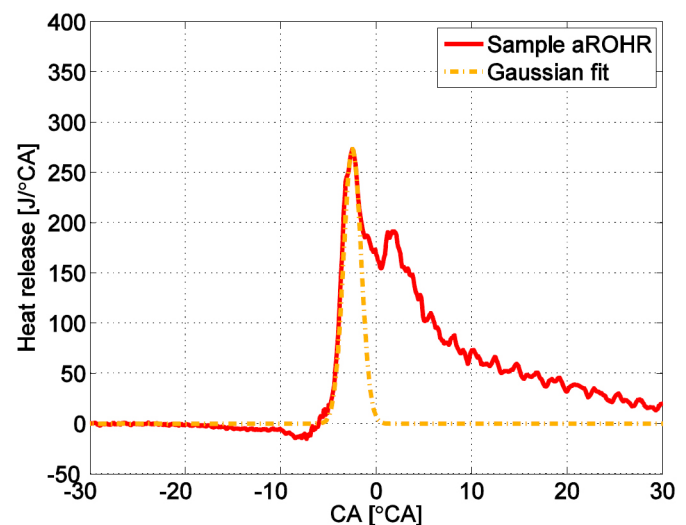


Figure 2. Rate of Heat Release and Gaussian profile as a function of crank angle degree. Gaussian fit is used to define the premixed fraction

Efficiencies

Combustion efficiency provides information about the completeness of combustion and it is used to derive thermal efficiency. In order to calculate the combustion efficiency all