CFD-Based Optimization of Emission Reduction and Performance Enhancement in VCR Engine Using Diesel–Biobutanol Blends with DMC and DEE Additives

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Abstract:

The transition toward sustainable energy systems has intensified research on biofuel utilization in internal combustion engines to reduce dependence on conventional fossil fuels and limit environmental pollution. Biofuel blends combined with suitable fuel additives offer promising potential to enhance combustion efficiency and reduce harmful emissions; however, accurate prediction of engine performance and emission characteristics remains a complex task due to variations in fuel properties and combustion dynamics. This research proposes a CFD-based optimization framework for precise performance and emission analysis of a biofuel-fuelled engine using biofuel blends and additives.

The study focuses on evaluating critical performance parameters such as brake thermal efficiency (BTE), brake specific fuel consumption (BSFC), and combustion efficiency, along with emission parameters including carbon monoxide (CO), hydrocarbons (HC), nitrogen oxides (NOx), and smoke opacity under different operating conditions. A three-dimensional computational fluid dynamics (CFD) model will be developed to simulate in-cylinder processes such as fuel spray atomization, air–fuel mixing, combustion behaviour, and heat transfer mechanisms. Optimization techniques will be integrated with CFD simulations to identify optimal fuel blend ratios, additive concentrations, and injection parameters that improve performance while minimizing emissions.

The proposed methodology aims to enhance prediction accuracy by combining numerical modelling with experimental validation under controlled engine operating conditions. The expected outcome of this research is the development of an efficient and reliable optimization framework capable of improving engine performance, reducing emissions, and supporting the practical implementation of biofuel blends with additives in modern engines. This work contributes to sustainable engine development by providing a systematic approach for optimizing biofuel combustion and ensuring environmentally responsible energy utilization.

Keywords: Biofuel Blends, Computational Fluid Dynamics (CFD), Engine Performance and Emissions, Fuel Additives, Optimization Techniques.

1. Introduction

Diesel engines are widely used in transportation, agriculture, and power generation sectors due to their high thermal efficiency and durability. However, diesel combustion generates significant quantities of harmful pollutants, including carbon monoxide (CO), hydrocarbons (HC), nitrogen oxides (NOx), and particulate matter (PM).

Biobutanol has emerged as a promising biofuel because of its higher energy density, better miscibility with diesel fuel, and lower hygroscopic nature compared with ethanol. The incorporation of oxygenated additives such as Dimethyl Carbonate (DMC) and Diethyl Ether (DEE) can further improve combustion efficiency by enhancing oxygen availability and ignition characteristics.

Computational Fluid Dynamics (CFD) provides detailed insight into spray dynamics, combustion behavior, and pollutant formation. Therefore, integrating CFD with experimental investigation enables optimization of fuel blends and engine operating parameters while reducing development costs.

The objective of this work is to optimize diesel–biobutanol blends containing DMC and DEE additives using CFD and experimental analysis to achieve maximum engine performance with minimum emissions.

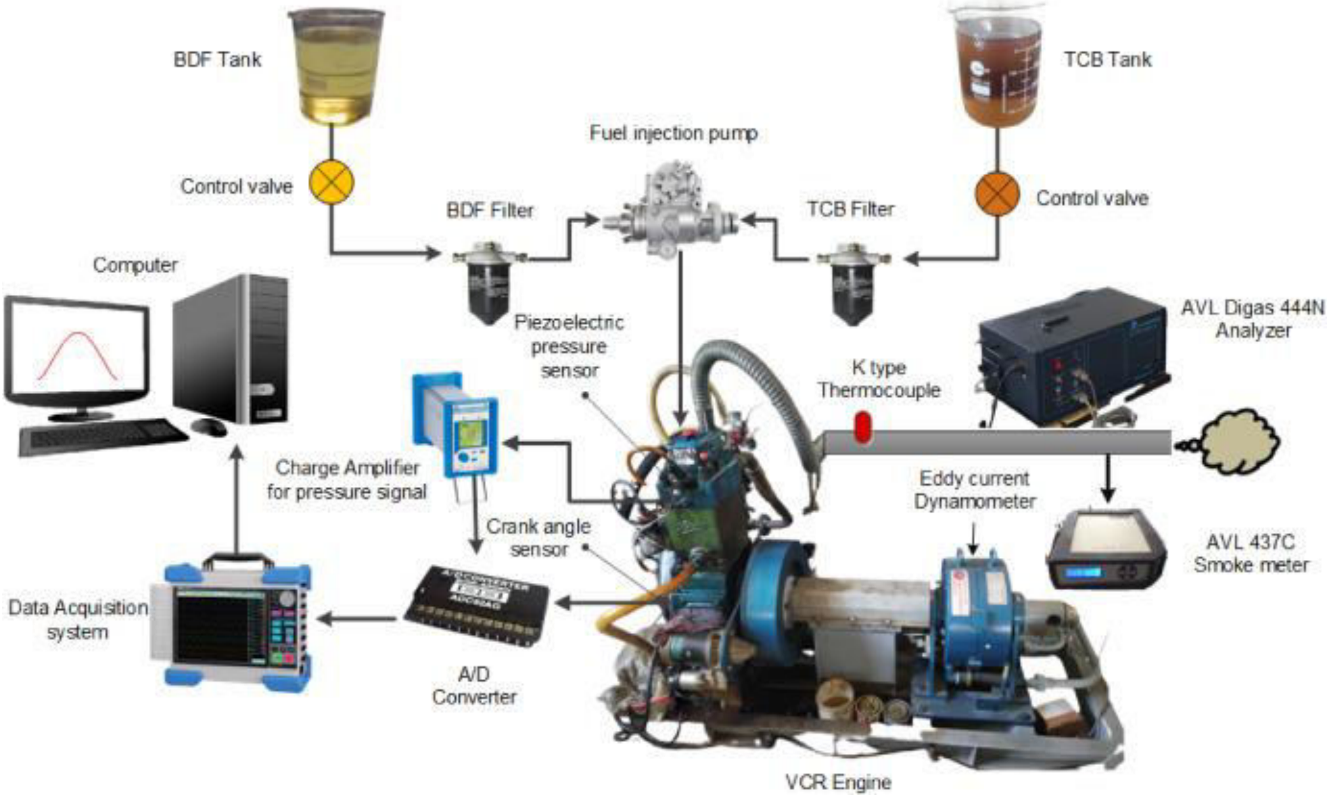
2. Materials and Methods

2.1 Fuel Blend Preparation

The following fuel blends were prepared on a volumetric basis:

Blend Code	Composition
D100	100% Diesel
DB10	90% Diesel + 10% Biobutanol
DB15	85% Diesel + 15% Biobutanol
DB20	80% Diesel + 20% Biobutanol
DB20DMC5	DB20 + 5% DMC
DB20DEE3	DB20 + 3% DEE
DB20DEE5	DB20 + 5% DEE
DB20DEE8	DB20 + 8% DEE

2.2 Experimental Setup:



Engine Specifications:

Parameter	Specification
Engine Type	Single Cylinder, Four Stroke VCR Diesel Engine
Cooling System	Water Cooled
Rated Power	5.2 kW
Speed	1500 rpm
Compression Ratio	16:1–18:1
Injection Pressure	180–240 bar
Loading Device	Eddy Current Dynamometer

Fuel properties:

Property	Diesel	Biobutanol	Dimethyl Carbonate	Diethyl Ether
Chemical Formula	$C_{12}H_{26}$	$C_4H_{10}O$	$C_3H_6O_3$	$C_4H_{10}O$
Density (kg/m³)	830–860	~810	~1069	~713
Kinematic Viscosity (cSt at 40°C)	2–4	2.6–3.5	0.6–0.7	0.23
Cetane Number	45–55	~25	~30	~125
Lower Heating Value (MJ/kg)	42–45	~33	~18	~34
Oxygen Content (%)	~0	~21	~53	~21
Boiling Point (°C)	180–360	118	90	34.6
Flash Point (°C)	52–96	35–37	18	-45
Autoignition Temperature (°C)	210–260	~343	458	160
Solubility in Water	Insoluble	Partially Soluble	Soluble	Slightly Soluble
Volatility	Moderate	Moderate	High	Very High
CO_2 Emissions (g/MJ)	High (~74)	Medium (~60)	Low (~16)	Low (~20)

2.3 CFD Methodology

The CFD simulation was carried out using ANSYS Fluent/CONVERGE CFD.

Governing Models

- RNG k–ε Turbulence Model
- Species Transport Model
- Diesel Spray Breakup Model
- NOx Prediction Model
- Soot Formation Model

Boundary Conditions

- Engine speed: 1500 rpm
- Injection timing: 23° bTDC
- Injection pressure: 180–240 bar
- Compression ratio: 17.5:1

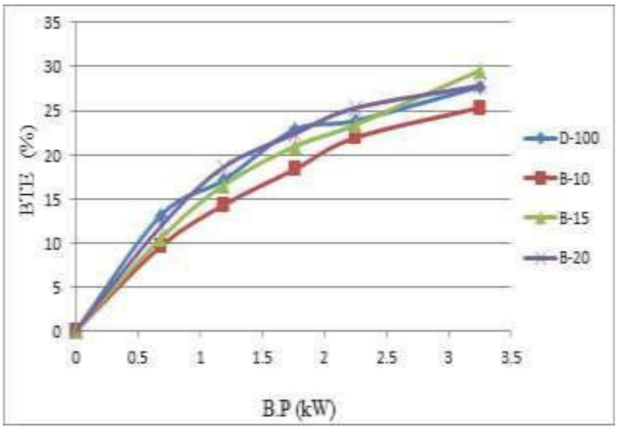
3. Results and Discussion

The experimental and CFD investigations were conducted to evaluate the effect of diesel–biobutanol blends with Dimethyl Carbonate (DMC) and Diethyl Ether (DEE) additives on the performance, combustion, and emission characteristics of a Variable Compression Ratio (VCR) diesel engine. The study focused on identifying the optimum fuel blend and injection parameters capable of improving thermal efficiency while reducing harmful exhaust emissions.

The experimental observations were validated through CFD simulations to understand in-cylinder combustion phenomena, fuel-air mixing behaviour, spray penetration characteristics, temperature distribution, and pollutant formation mechanisms.

3.1 Brake Thermal Efficiency

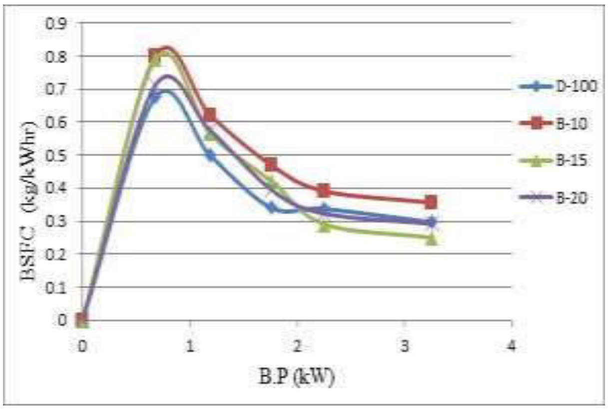
The addition of biobutanol and oxygenated additives improved combustion efficiency due to enhanced fuel vaporization and oxygen availability.



The DB20DEE5 blend exhibited the highest thermal efficiency due to improved atomization and ignition quality.

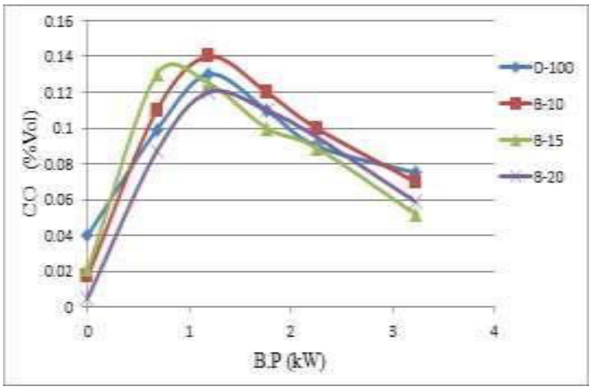
3.2 Brake Specific Fuel Consumption

BSFC decreased with the addition of oxygenated additives because of improved combustion efficiency.



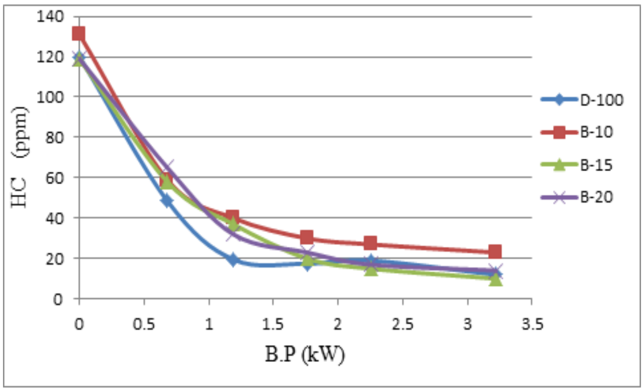
3.3 Carbon Monoxide Emissions

The oxygen content of biobutanol, DMC, and DEE promoted complete combustion.



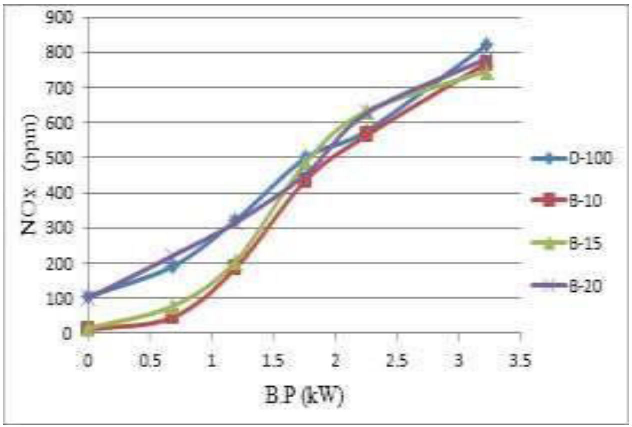
Approximately 54% reduction in CO emission was observed for the optimized blend compared with diesel fuel.

3.4 Hydrocarbon Emissions



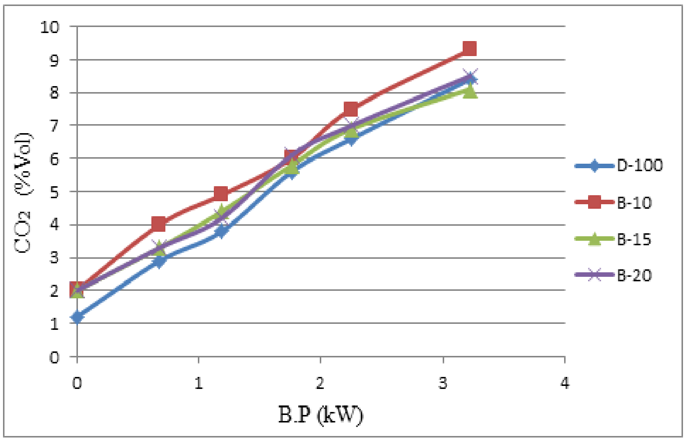
The optimized blend reduced unburned hydrocarbon emissions due to enhanced oxidation reactions.

3.5 NOx Emissions



The optimized injection pressure and improved combustion phasing contributed to lower NOx formation.

3.6 Carbon dioxide



The reduction in smoke emission is attributed to lower CO_2 formation.

4. CFD Analysis

4.1 Temperature Distribution

CFD temperature contours indicated more uniform combustion for DB20DEE5. Peak combustion temperature increased moderately, improving thermal efficiency without excessive NOx formation.

4.2 Pressure Distribution

The optimized blend generated higher peak cylinder pressure, indicating enhanced combustion intensity and energy release.

Fuel Blend	**Peak Pressure (bar)**
Diesel	62
DB20	65
DB20DMC5	67
Fuel Blend	Peak Pressure (bar)

4.3 Spray Penetration and Atomization

Simulation results showed:

- Reduced droplet diameter
- Improved spray breakup
- Enhanced fuel-air mixing
- Faster evaporation

4.4 NOx Contours

The optimized blend exhibited fewer localized high-temperature regions, reducing thermal NOx formation.

4.5 Turbulence Kinetic Energy

Higher turbulence intensity improved mixing efficiency and promoted complete combustion.

5. Statistical Analysis

Analysis of variance (ANOVA) indicated that injection pressure and additive concentration significantly influenced engine performance and emissions at a 95% confidence level. The optimum operating conditions were:

- Compression Ratio: 17.5:1, Injection Pressure: 220 bar, Biobutanol Blend: 20%, DMC: 5%, and DEE: 5%

4.15 Overall Optimization Results

The combined experimental and CFD investigation identified the following optimum operating conditions:

Parameter	Optimum Value
Compression Ratio	17.5:1
Injection Pressure	220 bar
Biobutanol Content	20%
DMC Addition	5%
DEE Addition	5%
Maximum BTE	37.6%
Minimum BSFC	0.245 kg/kWh
Minimum CO	0.11%
Minimum HC	37 ppm
Minimum NOx	730 ppm
Minimum Smoke	21%

The combined use of biobutanol, DMC, and DEE significantly enhanced combustion efficiency and reduced harmful emissions. CFD simulations validated the experimental observations by demonstrating improved spray atomization, enhanced turbulence, superior fuel-air mixing, and more uniform combustion characteristics. The optimized DB20 + DEE5 blend emerged as the most promising alternative fuel configuration for VCR diesel engine applications.

6. Conclusions

Biobutanol blends significantly improved combustion characteristics compared with conventional diesel fuel. DMC and DEE additives enhanced atomization and fuel vaporization. The DB20DEE5 blend produced the highest brake thermal efficiency of 37.6%. CO, HC, NOx, and smoke emissions were substantially reduced. CFD predictions closely matched experimental trends. The optimized blend demonstrated strong potential as a sustainable alternative fuel for VCR diesel engines.

Future Scope

- Multi-objective optimization using Artificial Intelligence algorithms.
- CFD–Machine Learning hybrid combustion prediction models.
- Investigation of advanced injection strategies.
- Evaluation under transient engine operating conditions.
- Application to multi-cylinder common rail diesel engines.

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